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ARGONNE NATIONAL LABORATORY

1991

FACULTY AND STUDENT

PROGRAMS

UNITED STATES DEPARTMENT OF ENERGY

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ARGONNE NATIONAL LABORATORY

Division of Educational Programs

The Division of Educational Programs is responsible for promoting, developing and facilitating educational and research interactions between Argonne National Laboratory and the academic community. Educatiònal activities at Argonne are intended to utilize the Laboratory's unique resources to further the scientific, technical and professional development of men and women for energy-related research and engineering careers. The activities of the Division are conducted for, and in partnership with, the U.S. Department of Energy and the academic community. The Division also conducts several important training programs for international participants. In discharging its responsibilities, the Division works with every scientifc division of Argonne, in addition to universities, colleges, several university consortia and the pre-college community.

Information contained in this book is intended to help familiarize potential faculty, teachers and students with Argonne National Laboratory research activities. Opportunities listed in this book are for the summer 1991 and the academic year 1991-1992.

We encourage applications for participation in our programs from faculty, teachers and students in the college, university and pre-college communities.

Robert W. Springer, Director
Argonne Division of Educational Programs

HOW TO USE THIS BOOK

This book is your guide to participation in research projects at Argonne National Laboratory. It contains descriptions of the various programs through which faculty and students may become involved in research at Argonne, as well as brief outlines of the research projects.

Consult the first section of the book for information about faculty and student programs. A table on pages 2 and 3 provides a summary of the available programs. More extensive descriptions follow.

The second section of the book contains a Catalog of Research Projects. Prospective participants should review the Catalog thoroughly to find the research projects of greatest interest to them. Notice that, in the left margin next to each project outline, the relevant academic disciplines are listed in *italics*. Regardless of your field of study, you may find an interesting project, to which you can make a valuable contribution, in any of the research divisions at the Laboratory - SO SCAN ALL PROJECT DESCRIPTIONS!! You can refer to the detailed index in the back of the book to ensure that you have not overlooked any projects in your field.

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MICHIGAN STATE U

Throughout the year, Argonne sponsors a number of activities designed to encourage undergraduates to pursue advanced degrees and research careers in science and engineering. The Graduate School Fair, held each October, helps students from the five-state region identify the graduate program which best meets their needs and interests. In attendance at last year's Fair were faculty representatives from over 80 of the country's leading graduate programs.

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RESEARCH
PARTICIPATION
PROGRAMS

ARGONNE NATIONAL LABORATORY - PROGRAM SUMMARY

Program	Term	Eligibility
Faculty Research	Summer, 12 weeks or fewer	Full-time faculty at accredited U.S. colleges or universities.
Faculty Research Leave	9 to 12 months	Full-time faculty at accredited U.S. colleges and universities. Must be in receipt of sabbatical leave or other appropriate award.
Science and Engineering Research Semester	Academic Term (Sept.-Dec.) (Jan.-May)	College juniors and seniors. Minimum GPA 3.0/4.0, U.S. citizens or permanent resident aliens (PRA).
Summer Research	11 weeks (June-Aug.)	Students must have completed sophomore year; Minimum GPA 3.0/4.0; U.S. citizens or PRA.
Laboratory-Graduate Appointments	1 year, renewable	Graduate students at U.S. colleges and universities.
Thesis Parts Appointments	Variable, up to 6 months	Graduate students at U.S. colleges and universities.
Guest Graduate Appointments	Variable	Graduate students at U.S. colleges and universities.
Cooperative Education (Alternating Co-ops)	4 quarters or 3 semesters of work	Students in engineering or science at U.S. colleges and universities.
(Parallel Co-ops)	6 months to 2 years	Students in engineering or science at Chicago area colleges and universities.
Short-term Appointments	Variable, up to 6 months	Students at U.S. colleges and universities.
Pre-College (For Chicago Area, Summer Only)	8 weeks	High school graduates.
	4-5 weeks	Students with 2 years high school.
	1 week	Students with 1 year high school.
	8 weeks	High school science and math teachers.
Chicago Science Explorers (In partnership with Chicago cultural and scientific institutions)	Academic year	Teachers and classes in the Chicago Area with emphasis on minority students.
Regional Instrumentation Sharing Program	Typically 1-3 days	U.S. college faculty and students who need access to advanced instrumentation available at Argonne.
Workshops, Institutes and Conferences	Variable	Faculty and students at colleges and universities.
Postdoctoral	Variable	Recent doctoral graduates.
Visiting Scientist Appointments	Variable	Faculty at U.S. and foreign colleges and universities.

Payment	Application Deadline	Description	Page No.
Stipend (based on academic salary, max. $1200/wk); Travel*	January 10	Collaborative research; in many cases resulting in publications and improved chances of receiving on-campus federal funding.	4
1/2 academic salary (+ summer); Relocation costs negotiable	6-9 months prior to desired start date		5
$200/week; Housing; Travel*	March 15 for fall October 20 for spr.	Research internship. Staff supervision. Advanced coursework. Seminars	7
$200/week; Housing; Travel*	February 1	Research internship. Staff supervision. Seminars	6
Stipend; up to $3500/year tuition	None	Students carry out thesis research at Argonne under staff supervision.	9
Per diem; Travel	None	Students carry out portions of their thesis research at Argonne.	10
None	None	Provides graduate students access to Argonne resources.	10
$8/hour and up	None	Alternating terms; full-time work at ANL, then full-time study on campus.	12
$8/hour and up	None	Part-time work at ANL while full-time study on campus.	
Competitive salaries	None	Appointees carry out assigned technical tasks.	12
$175/week	March 20	Participate in scientific research at ANL.	10
$60/week	March 20	Materials science and nuclear science.	
Lunch provided	March 20	Materials science instrumentation.	
$500/week	December 15	Participate in scientific research at ANL.	
Inservice stipend and classroom materials for teachers; Bus service for class groups on field trips	Will be announced in the fall and in the spring	Teachers are trained in the use of videos, classroom activities and field trip activities. Students meet scientists and conduct experiments. Program encourages students to consider science careers.	11
None	None	Instrumentation for research and for teaching undergraduate and pre-college students.	13
None	None	Various meetings about research topics at ANL.	13
Competitive salaries	None	Provides exceptional research opportunities.	14
Academic salary	None	Temporary appts. for interaction and research.	14

*Roundtrip, if greater than 100 miles

GENERAL INFORMATION

Argonne National Laboratory offers college and pre-college faculty and students many opportunities to participate in the ongoing research programs of the Laboratory. Approximately one hundred faculty members and five hundred students are involved annually. The program, administered by Argonne's Division of Educational Programs, is funded by the U.S. Department of Energy, Office of Energy Research, through its University/DOE Laboratory Cooperative Program and through its research divisions.

Faculty and student research participation is welcomed in the basic PHYSICAL and LIFE SCIENCES, MATHEMATICS, COMPUTER SCIENCE and ENGINEERING as well as in a variety of applied research areas relating to COAL, CONSERVATION, FISSION, FUSION and ENVIRONMENTAL TECHNOLOGY. This booklet contains descriptions of the research conducted by groups in Argonne's research divisions. The academic disciplines utilized in each research area are noted in italic next to each description; major equipment items used by each project are also listed.

Argonne is an Equal Opportunity Employer (M/F) committed to Affirmative Action. Applications from physically handicapped individuals are welcomed.

FACULTY PROGRAMS

Two programs enable college/university faculty to take part in the Laboratory's research programs:

FACULTY RESEARCH PARTICIPATION (SHORT-TERM APPOINTMENTS)

APPLICATION DEADLINE (Summer Program): January 11, 1991

Faculty participants in the program typically spend 10-12 weeks collaborating with an Argonne staff scientist or engineer on an existing Argonne project of interest to the faculty member. The research experience is augmented by seminars, independent study and other appropriate activities. Appointments are made principally for the summer; however, similar arrangements can be made during the academic year (no application deadline).

An appointee must be a full-time faculty member of an accredited U.S. college or university, and must have a commitment to continue in teaching and research as a career. The applicant's objectives for the Argonne appointment should be clearly specified, and these objectives must be endorsed by the applicant's department head or dean.

Financial support is available to full-time faculty of U.S. academic institutions. Participants will be provided with a stipend based upon their academic-year salary (up to a maximum of $1200 per week) and travel between their home and Argonne, if the round-trip distance is greater than 100 miles.

Application materials can be obtained by writing to:

Division of Educational Programs
Faculty Research Participation Programs
Argonne National Laboratory
Argonne, Illinois 60439-4845
(708) 972-3365

FACULTY RESEARCH LEAVE (SABBATICAL LEAVE)

APPLICATION DEADLINE: None

Faculty members spend their sabbatical leave, typically 9-12 months, at the Laboratory. Over 120 appointments have been made since the program's inception in 1980.

The Faculty Research Leave Program is intended to provide mutual benefits to the faculty members and the Laboratory. In addition to bringing about fruitful research activity, it should give Argonne scientists and engineers and visiting faculty opportunities to develop a strengthened rapport and deepened appreciation of mutual needs and interests pertaining to research development and to catalyze the formation of continuing research partnerships and collaborations.

Interactions of faculty with students in the research programs is strongly encouraged. This can take the form of research collaboration as well as more conventional interactions such as seminars and teaching. Also, when funding is available, faculty can involve qualified student(s) from their home campus in their Argonne research program.

Appointments will normally be for an academic or a calendar year, extendable, if mutually agreed upon by the faculty member, the home institution and Argonne. To be eligible for the appointment, a faculty member must be in receipt of a sabbatical leave award (or other appropriate award) from his/her university, have the approval of the appropriate university administrator to accept the Argonne appointment, and have demonstrated accomplishment in an area of research and/or development relevant to research at Argonne.

During his/her Faculty Research Leave appointment the faculty member will remain on the payroll and under the fringe benefits of the university. Typically, Argonne will reimburse the university for 50% of salary and fringe benefits for the academic-year (9 months) and full salary and fringe benefits for the summer period (3 months). In addition, the Laboratory may, by direct payment to the faculty member, negotiate reimbursement for certain travel, moving and housing expenses.

Argonne desires that the expression of interest in Faculty Research Leave participation by an individual faculty member, along with university endorsement of such participation, be transmitted to the Faculty Program Leader, Argonne Division of Educational Programs. Initial expressions of interest should include a curriculum vitae, a publication list and a brief statement of the research interests of the faculty member. There should also be an indication by the responsible university official that the faculty member is eligible to receive a sabbatical or other appropriate award.

STUDENT PROGRAMS

The student research programs at Argonne are educational experiences designed to provide participants with the opportunity to study and carry out research at the frontiers of their fields of interest. Participation in the program takes the form of an individual collaboration with an Argonne staff member in some part of an ongoing project of interest to the student participant.

Three programs exist at Argonne in which college/university students may obtain research experience. These are the Summer Research Participation (SRP) Program, the Science and Engineering Research Semester (SERS), and the Graduate Student Thesis Research Program. While specific details for SRP and SERS are given below, a student will generally spend the first week of his/her Argonne experience with an Argonne staff member devising a research strategy. For the next few weeks the supervisor will provide considerable program assistance and guidance. Subsequently, the student will be expected to perform relatively independently and complete the project on his/her own initiative. Each student is required to submit a mid-term progress report and a final research report.

To be eligible for SRP or SERS, a student must:

- have a grade point average of at least 3.0 on a 4.0 scale, and
- be a U.S. citizen or permanent resident alien.

Selection for any program is based upon a student's academic record, statement of interests, and his/her faculty member recommendations.

SUMMER RESEARCH PARTICIPATION PROGRAM

APPLICATION DEADLINE: February 1, 1991

The Program:

The Summer Research Participation Program extends for an eleven-week period which begins in early June and runs through mid-August. In addition to their research activities, participants are expected to attend a series of seminars and tours dealing with current topics in science and engineering.

Normally, participants in the summer program must have completed their sophomore year and not more than their first year of graduate study. While students must generally have matriculated status, science or engineering graduates who have been out of college for no more than one year will also be considered for the program.

Financial Assistance:

During the appointment period, participants receive a stipend of $200/week and complimentary housing or a housing allowance+. All housing arrangements for single students are handled by Argonne's Division of Educational Programs. Transportation expenses are reimbursed for one round-trip between the Laboratory and the participant's home or university for round-trip distances greater than 100 miles. If travel is via personal auto, reimbursement is at a rate of 24 cents per mile, with the total not to exceed coach-class airfare.

+Stipends and complimentary housing are considered taxable income by the IRS.

Application Procedure:

An application packet can be obtained by writing to:

Division of Educational Programs
Student Research Programs
Argonne National Laboratory
Argonne, Illinois 60439-4845
(708) 972-4579

Once completed, the application form should be returned to the above address. The Student Evaluation Forms found in the application packet should be given to faculty members with whom the applicant has had frequent contact. The faculty member should mail the evaluation form directly to the Division of Educational Programs. These forms must be returned to complete your application file.

SCIENCE AND ENGINEERING RESEARCH SEMESTER

APPLICATION DEADLINES: 1991 Fall Program -- March 15, 1991
1992 Spring Program -- October 20, 1991

The Program:

As part of a recent, nationwide Department of Energy initiative, the Science and Engineering Research Semester offers challenging opportunities for students selected nationally for participation in energy-related research during the academic year. The program enhances the historic collaboration between the university community and the national laboratories and strengthens the quality of science, mathematics, and engineering research and education.

The core of the academic-year SERS Program is the student research experience. As such, the student is expected to devote at least 35 hours per week to research on a specific project under the mentorship of an Argonne staff scientist. In addition to a mid-term and final report, each student will also be required to present a brief seminar at Argonne on his/her research project.

In addition to the research experience, courses which should accommodate the needs and interests of a majority of the student participants will be available. Information on the specific courses to be offered during a particular term can be obtained by writing to the Division of Educational Programs or by calling the Argonne SERS coordinator at (708) 972-4579.

Should a student require a special course not offered as part of the regular program, he/she will be allowed to substitute a course offered by a regional university. In this case, arrangements MUST be made by the student well in advance of his/her stay at Argonne. Students whose special needs are not covered by any of the above options may arrange with their home campus faculty for independent study to be conducted at Argonne under the supervision of one of the Argonne staff.

In addition to the above activities, Argonne has integrated into its program a number of special features and activities. During the Fall term, SERS participants have the opportunity to attend the Argonne Graduate School Fair in Science and Engineering. At this Fair students have the chance to talk, one-on-one, with faculty representatives from some of the finest graduate schools in the U.S. On October 6, 1990 we will have over 100 departments represented, including: Princeton, Yale, The University of Chicago, Georgia Tech, to name a few. In the Spring term, a number of the program's students are selected for an expense-paid trip to make a presentation on their Argonne research at the annual undergraduate conference sponsored by the National Council on Undergraduate Research. Last year, 12 Argonne students attended the Conference at Union College in Schenectady, New York. In addition to the above special activities, many cultural and scientific resources exist in the greater Chicago area. Trips to the Aquarium, Planetarium, Fermi National Accelerator Laboratory, Art Institute of Chicago, Museum of Science and Industry, etc., are also available.

Academic Credit:

Students are encouraged to seek academic credit from their home institutions for their SERS experience. Recommended credit is 12-16 semester hours or the equivalent: Interdisciplinary Seminar, 1 credit; Advanced Course, 3 credits; Research, 8-12 credits. The exact number of credits a student receives must be determined by the student in consultation with the student's departmental chairperson or advisor. DEP is willing to provide whatever assistance it can in helping a student arrange for academic credit.

Periods of Appointment:

In order to provide the student with maximum scheduling flexibility, a variety of terms and term lengths have been developed. These include:

Single Terms:

Fall (15 weeks)
Early September through mid-December
Application Deadline: March 15, 1991

Spring (15 weeks)
Mid-January through mid-May
Application Deadline: October 20, 1991

Multiple Terms:

Summer-Fall (26 weeks - 1 week leave (optional))
Early June through mid-December
Application Deadline: February 1, 1991

Spring-Summer (30 weeks - 2 week leave (optional))
Mid-January through mid-August
Application Deadline: October 20, 1991

Financial Assistance:

During the appointment period, participants receive a stipend of $200/week and complimentary housing or a housing allowance+. All housing arrangements for single students are handled by Argonne's Division of Educational Programs. Transportation expenses are reimbursed for one round-trip between the Laboratory and the participant's home or university for round-trip distances greater than 100 miles. If travel is via personal auto, reimbursement is at a rate of 24 cents per mile, with the total not to exceed coach-class airfare.

+Stipends and complimentary housing are considered taxable income by the IRS.

Costs:

As all credits will be awarded directly by the student's home institution, students will pay the appropriate tuition to their home university. IN MOST CASES, STUDENTS RECEIVING FINANCIAL AID REMAIN ELIGIBLE FOR THEIR SCHOOL'S FINANCIAL AID PROGRAM. STUDENTS SHOULD CONSULT THEIR FINANCIAL AID OFFICER WELL IN ADVANCE.

Application Procedure:

As the Argonne Science and Engineering Research Semester is part of a national, six-laboratory Department of Energy program, application materials may be obtained from either the central Washington office:

Science and Engineering Research Semester
U.S. Department of Energy
Office of Energy Research, Room 3F-061
Forrestal Building
1000 Independence Avenue, S.W.
Washington, DC 20585
(202) 586-8949

or by writing to Argonne directly:

Science and Engineering Research Semester
Division of Educational Programs
Argonne National Laboratory
Argonne, IL 60439-4845
(708) 972-4579

GRADUATE STUDENT PROGRAMS

LABORATORY-GRADUATE PARTICIPANTSHIP APPOINTMENTS

Laboratory-Graduate Participantship (Lab-Grad) appointments are available for qualified graduate students at U.S. universities who wish to carry out their thesis research at Argonne National Laboratory under the co-sponsorship of an Argonne staff member and a faculty member. The university sets the academic standards and awards the degree. In practice, the participation by the faculty member varies from full partnership in the research to general supervision. The Argonne staff sponsor undertakes to keep the faculty sponsor informed about the student's progress and he/she attends the thesis defense.

Research may be conducted in the basic physical and life sciences, mathematics, computer science, and engineering as well as in a variety of applied areas relating to conservation, environment, fission and fusion energy, and other energy technologies.

Lab-Grad appointments are for a one-year term with annual renewals being contingent upon satisfactory performance by the appointee. Appointments usually commence when the student begins full-time thesis research at Argonne after having completed all other academic requirements. In certain cases students may be awarded support for pre-thesis studies on campus, provided that they intend to carry out their thesis research at Argonne.

Support of a Lab-Grad appointee consists of a stipend, tuition payment up to $3,500 per year and certain travel expenses. In addition, the student's faculty sponsor may receive payment for limited travel expenses.

An application for a Lab-Grad appointment may be submitted at any time during the year and an appointment may commence at any time. A completed application should be submitted at least one month prior to any proposed starting date but earlier application submission is advantageous because the availability of Lab-Grad appointments is limited by funding constraints.

Mutual interest in an area of research by the student and the Argonne staff sponsor is essential for the successful arrangement of a Lab-Grad appointment. To help the parties gauge their mutual interest a limited number of temporary appointments are available for qualified graduate students so that they may work with an Argonne staff member and become familiar with his/her research program. These temporary appointments have a tenure of three months and support consists of a per diem payment to help defray the cost of living away from home, plus travel expenses.

Students wishing to submit applications for a Lab-Grad appointment or a temporary appointment are advised to identify and make initial contact with a possible Argonne staff or research division sponsor.

THESIS PARTS APPOINTMENTS

Thesis Parts Appointments support qualified graduate students who wish to visit Argonne for periods from a few days to a few months, so that they may utilize special Laboratory facilities or capabilities during the course of their thesis research. Support consists of a per diem amount to help defray the cost of living away from home, plus transportation. Application is best made through an Argonne staff person or research Division appropriate to the proposed activity.

GUEST GRADUATE APPOINTMENTS

Guest Graduate Appointments are available for qualified graduate students who show that access to Argonne National Laboratory will be beneficial to their thesis research and to Argonne programs. A Guest Graduate is given a gate pass, usually for one year, and the student may visit Argonne whenever appropriate. A Guest Graduate receives no stipend or payment of any kind from the Laboratory.

For application materials and further information about any of these graduate student programs, or for assistance in identifying an appropriate Argonne staff member, write to:

Division of Educational Programs
Graduate Student Program Office
Argonne National Laboratory
Argonne, Illinois 60439-4845
(708) 972-3371

PRE-COLLEGE PROGRAMS

The Pre-College Programs can be divided into two different types: (1) research participation activities at the Laboratory and (2) outreach activities. Both of these activities involve pre-college students and pre-college teachers. The range of programs is listed below:

RESEARCH PARTICIPATION

High School Student Research Apprenticeship:

Each summer a five-week program for approximately 40 Chicago-area students between their sophomore and junior year is conducted in which these students progress through laboratory exercises using sophisticated instrumentation and learn about the scientific method.

Scientific Instrumentation:

A one week program for Chicago-area high school juniors in Scientific Instrumentation is conducted twice each summer. The program introduces students to a variety of scientific instruments used in measurements and provides them an opportunity to participate in several different experiments in small groups.

Pre-College Research Participation:

Thirty to forty Chicago-area high school seniors are assigned to work individually or in pairs with research scientists at the Laboratory.

DOE Honors Program:

A national DOE Honors Program is conducted annually for two weeks in the summer. Six students are selected by each state and are assigned to different DOE Laboratories for a research and enrichment experience. The Argonne program emphasizes superconductivity and materials science.

Explorer Post Program:

This series of weekly evening lectures and laboratory tours operates during the school year. It is designed to acquaint sophomore, junior, and senior high school students with the fields of science and engineering and to encourage them to pursue careers in these areas. Over 150 students from more than 20 high schools participate each year.

Science Bowl:

The Argonne Science Bowl is a tournament-style team quiz competition designed to provide recognition to students who have a special interest in science and mathematics. Thirty-two school teams participate in the competition answering questions posed by Argonne scientists. Trophies are awarded to the first, second, and third place teams.

Teacher Research Associates:

Each Summer for eight weeks teachers from both the Chicago area and throughout the country participate in research with scientists at the Laboratory. Each teacher typically takes some of his research experience into the classroom during the next year.

CLASSROOM AND OUTREACH ACTIVITIES

Regional Instrumentation Sharing Program:

The Regional Instrumentation Sharing Program offers many teachers and their students access to a laboratory of research instruments maintained by the Division of Educational Programs for use in workshops and for visiting classes. Many teachers also attend in-service workshops on topics such as superconductivity. The workshops on superconductivity are supported by the NSF Superconductivity Center and by the State of Illinois. Other workshops and conferences are held annually for teachers and Chicago area students.

Argonne Community of Teachers:

The Argonne Community of Teachers (ACT) is an organization of Chicago-area teachers led by a group who have formerly participated in some of the Argonne educational programs. A committee made up of ACT members conducts workshops and conferences for teaching colleagues in the Chicago area. The conferences and activities of the group are open to any teacher in the Chicago area.

The Chicago Science Explorers Program:

This program offers to teachers a package containing a videotape created by Bill Kurtis of WBBM-TV (CBS), teaching guides and classroom activities supporting the tape, and free transportation for a field trip to one of a number of sites. The program is designed to encourage students, especially minorities, to consider a career in science. The program is supported by a group of institutions called the Chicago Science Explorer Partners and includes: Field Museum of Natural History, Adler

Planetarium, Shedd Aquarium, Chicago Academy of Sciences, Museum of Science and Industry, Lincoln Park Zoo, Brookfield Zoo, Fermi Accelerator Laboratory, and Argonne National Laboratory. The project is supported by Chicago State University and the University of Chicago Laboratory School. Teachers participate in the program by applying for in-service training sessions for each videotape.

Information on any of the Pre-College programs can be obtained by writing to:

Division of Educational Programs
Pre-College Programs
Argonne National Laboratory
Argonne, Illinois 60439-4845
(708) 972-3373

OTHER FACULTY AND STUDENT PROGRAMS

TEMPORARY EMPLOYMENT FOR COLLEGE/UNIVERSITY STUDENTS

Short-Term Appointments:

In addition to research participation opportunities, Argonne offers temporary employment appointments to college/university students. These appointments, made primarily during the summer months, are designed to provide the Argonne scientific and engineering staff with technical assistance. Rather than designing their own research program, temporary employees are assigned specific technical tasks. Student-level temporary employees earn a salary, are expected to possess the skills required to do the assigned task when they arrive, and do not participate in the seminar series and field trips. Understanding of the scientific basis for the temporary employee's work is generally not emphasized. Students applying for temporary employment should use the research participation application form, clearly marking the temporary employment box. **Application deadline for Summer Temporary Employment is February 1, 1991**.

Cooperative Education:

Appointments made primarily during the academic year, are available to students after completion of 2, 3 or 4 semesters. Salaries are competitive and are based upon the number of terms of study and co-op work periods completed. Applications should be submitted through the student's university Cooperative Education Office, and may be submitted at any time.

Argonne has two types of CO-OP Programs: Alternating (full-time work, followed by full-time school) and parallel (part-time work concurrent with full-time school). About 60% of the students employed are computer science majors, 30% are engineers (chemical, electrical, ceramics, material science and nuclear) and the balance are chemistry, physics and economics majors. The following Argonne Divisions are arranged by the largest number of CO-OP students they employ: Energy and Environmental Systems, Chemical Technology, Physics, Materials and Components Technology, Reactor Analysis and Safety, Computing Services and Materials Science.

A student who is employed in the CO-OP Program is expected to work a minimum of one year as a parallel CO-OP or 3 semesters as an alternating CO-OP. Students who are interested in shorter lengths of employment should apply for "Temporary Employment" described in the preceding section. Undergraduate CO-OP opportunities are available to students while they are attending graduate schools in the Chicago Area. The application packet can be obtained by writing to:

Division of Educational Programs
CO-OP Programs
Argonne National Laboratory
Argonne, Illinois 60439-4845
(708) 972-5448

REGIONAL INSTRUMENTATION SHARING PROGRAM

The purpose of this program is to provide instrumentation for college and university faculty in cases where adequate resources are not available to them. A number of qualified researchers from academic institutions will be given access to selected instrumentation at Argonne National Laboratory. Faculty participants are encouraged to involve their students in research work carried out under this program. In the event that these interactions lead to collaborative research with Argonne staff, follow-up grants are available through the Cooperative Research Development Program of the Division of Educational Programs.

Instrumentation is available through research divisions in the Physical, Engineering, Energy, Environmental and Biological Sciences.

The Division of Educational Programs operates an undergraduate teaching laboratory where a large variety of spectroscopic and analytic instrumentation is available to college and university groups. The purpose of the facility is to augment hands-on experience with advanced instrumentation in the areas of nuclear physics, physical and organic chemistry, materials science and biology.

Argonne National Laboratory also operates major research user-facilities that are available, through user-committees, to qualified researchers from industry, academia and other national laboratories.

For further information, please address inquiries to:

Division of Educational Programs
Regional Instrumentation Sharing Program
Argonne National Laboratory
Argonne, Illinois 60439-4845
(708) 972-3373

WORKSHOPS, INSTITUTES AND CONFERENCES

Workshops, Institutes and Conferences are offered throughout the calendar year by the Division of Educational Programs and the appropriate programmatic research division. These meetings focus on the research strengths of the Laboratory.

These meetings, under the umbrella of the Waterfall Glen Series, present a visible and coherent picture of DOE research programs to college and university faculty. Many of these meetings are focused at college and university faculty in order to provide a tutorial atmosphere by which experts from the Laboratory, universities and industry provide state-of-the-art information in an informal atmosphere. Through this forum, we hope to motivate interactions among the academic community and Laboratory staff.

For further information on the workshop program, please address inquiries to:

Division of Educational Programs
Workshops, Institutes and Conferences
Argonne National Laboratory
Argonne, Illinois 60439-4845
(708) 972-3373

POSTDOCTORAL APPOINTMENTS

Postdoctoral research appointments are available at the Laboratory, and provide exceptional research opportunities for individuals who have recently earned doctoral degrees and whose research interests are pertinent to the broad programs of the Laboratory. For further information, please address inquiries to:

Human Resources Department
Professional Placement
Argonne National Laboratory
Argonne, Illinois 60439-4872
(708) 972-2974

VISITING SCIENTIST PROGRAM

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CATALOG OF RESEARCH PROJECTS AT ARGONNE NATIONAL LABORATORY

ARGONNE-WEST (AW)

Argonne National Laboratory's Argonne-West (ANL-W) site is located at DOE's Idaho National Engineering Laboratory (INEL). The site represents one of the most advanced in the nation for the development of liquid-metal-cooled fast breeder reactors. The four major facilities and one activity at ANL-W play a major role in the nation's Liquid Metal Breeder Reactor Program. These are: Experimental Breeder Reactor-II (EBR-II), the Zero Power Plutonium Reactor (ZPPR), the Transient Reactor Test Facility (TREAT), and the Hot Fuel Examination Facility (HFEF) complex and the Integral Fast Reactor (IFR) activity. A brief description of each of these activities is below. Backup facilities such as chemistry and nondestructive analysis laboratories are also operated at the ANL-W site. Research activities are widely varied and many different types of projects are available: sodium and water analysis, sodium-void reactivity determinations, radiochemistry, materials research, LMR safety and analysis, operational problem-solving, shielding calculations, in-cell equipment design, and reactor physics, to name a few.

100 EXPERIMENTAL BREEDER REACTOR-II

Comp. Sci.
Elec. Engr.
Mat.. Sci.
Math
Mech. Engr.
Nucl. Engr.
Phy.

EBR-II is a sodium-cooled fast breeder reactor with a full-power output of 62.5 megawatts thermal. The reactor was brought to "wet" criticality, with the core submerged in liquid sodium, in November 1963. The present electrical output of 19 megawatts (19,000 kilowatts) is fed into the power grid of the INEL. The original purpose of EBR-II was to demonstrate the feasibility of using a liquid-metal-cooled fast breeder reactor and its auxiliary systems as a power station. The primary advantage of a breeder reactor is its ability to produce more fissionable material than it consumes. A fuel reprocessing plant was constructed adjacent to EBR-II and reprocessed about 35,000 EBR-II fuel elements successfully before the facility was converted to other uses. EBR-II has successfully demonstrated the feasibility of breeder reactors in power stations. The present mission of EBR-II is that of an irradiation facility for testing improved breeder fuels and materials and a test facility for determining plant dynamic response to off-normal events of the kind that could reasonably be expected in future sodium-cooled fast reactors. This work also includes development and testing of computer-based diagnostic and control systems. The irradiation tests are essential for the selection of materials and the development of reliable and economic fuels for large breeder reactors. The core loading of EBR-II has been changed to accommodate experimental subassemblies. As many as 1200 samples (60 subassemblies) of reactor fuels and reactor structural materials have been under test during some runs. As a sodium-cooled reactor, EBR-II also serves as a valuable facility for improving the technology of dealing with sodium. In 1986 tests were completed demonstrating that EBR-II will shut itself down safely on a complete loss of coolant pumping power with no operator or safety system protective action. These tests and other planned R&D research at EBR-II will provide significant input for the design of an inherently safe nuclear power plant in the future.

101 ZERO POWER PHYSICS REACTOR

Comp. Sci.
Math.
Mech. Engr.
Nucl. Engr.
Phy.

The Zero Power Physics Reactor is a unique critical-experiment facility operated by Argonne National Laboratory to obtain fast-reactor physics information. The ZPPR is the world's largest and most flexible critical facility, capable of accommodating full-scale mockups of breeder reactors that eventually may be found in power plants capable of producing more than 1,000,000 kilowatts of electricity. Two general types of experiments are conducted in the ZPPR. One kind consists of basic studies that check the accuracy of methods of calculations used by reactor designers. The second kind consists of studies that are made to proof-test an actual reactor design. Measurements conducted as part of each experiment investigate neutron and gamma-ray intensities as functions of time, space, and energy, together with studies of factors influencing safety, economics, and reactor control. ZPPR began operation on April 18, 1969. Early ZPPR studies included a mockup core of the Fast Flux Test Facility. From 1970 to 1982, the facility was used primarily to support the U.S. breeder reactor demonstration project -- the 375,000 kilowatt-electric Clinch River Breeder Reactor. Other experiments have tested design concepts for 700,000 to 900,000 kilowatt-electric breeder reactors. More recently, the facility has tested 100 to 300 kilowatt-electric space reactors.

102 TRANSIENT REACTOR TEST FACILITY

Comp. Sci.
Math.
Nucl. Engr.
Phy.

TREAT is an air-cooled thermal reactor that was designed to test reactor fuels under conditions simulating various types of nuclear excursions. The reactor was first made critical in February 1959, and the reactor building underwent a major expansion in 1982 as part of a major upgrade. Early experiments involved safety studies for the Experimental Breeder Reactor-II (EBR-II), and metal-water-reaction tests for water-cooled-reactor safety programs. Currently, transient experiments are directed to answering safety questions related to the liquid-metal reactor and the new production reactors. The TREAT reactor also provides a neutron radiography facility, and is operated in the steady-power mode to obtain neutron radiographs supporting experimental programs.

103 HOT FUEL EXAMINATION FACILITY

Chem. Engr.
Comp. Sci.
Elec. Engr.
Math.
Mech. Engr.
Met. Engr.
Mat.. Engr.
Nucl. Engr. *Phy.*

HFEF consists of hot cells, support facilities, and equipment for handling and examining irradiated test specimens, and for preparing and packaging irradiated materials for shipment to other examination or disposal facilities. HFEF includes two facilities -- HFEF/North and HFEF/South. Each facility contains two shielded hot cells, one with an inert-gas (argon) atmosphere and the other with an air atmosphere. The HFEF/South facility adjoins the EBR-II reactor building and was originally constructed to develop and demonstrate remote reprocessing and refabrication of EBR-II fuel. In 1968, HFEF/South completed its original mission and was equipped for examination of irradiated materials for breeder reactors. HFEF/S is now being modified to demonstrate the reprocessing phase of the Integral Fast Reactor (IFR) program. HFEF/North became operational in 1975. This modern hot cell facility accommodates large irradiated components and provides highly reliable containment of alpha-emitting radioactive particulates. Examination capabilities include gamma-scanning, profilometry and other dimensional measurements, weight determinations, metallography (including scanning-electron microscopy), visual and photographic examinations, eddy-current testing, and neutron radiography and tomography. A 250 kW TRIGA reactor located beneath the hot cell provides the two neutron beams used for radiography.

104 FUEL CYCLE ENGINEERING

Chem. Engr.
Comp. Sci.
Elec. Engr.
Mat. Sci.
Mech. Engr.
Met. Engr.
Mfg. Engr.

Fuel Cycle Engineering research and development activities are in support of the Argonne Integral Fast Reactor (IFR) concept. The IFR is an advanced reactor concept which utilizes a pool-type liquid-metal-cooled and metal-fueled reactor with a small fuel-reprocessing facility co-located on the same plant site. The reactor with metal fuel provides inherent safety and construction cost savings.

As compared with oxide fuels, metal fuel reprocessing can be accomplished at a significantly lower cost in a much smaller facility with less equipment. The equipment is highly mechanized with robotic operation and maintenance, and the process is automated under integrated computer-control. At Argonne-West, metal-fuel reprocessing and refabrication technology is being developed and will be demonstrated using fuel irradiated in the EBR-II facility. Activities include designing, equipping, and reactivating a major remote-operating hot-cell facility, HFEF/S, with complete metal-fuel reprocessing-and-refabrication systems to demonstrate the metal-fuel cycle. Studies and concept development for a commercial-size co-located metal-fuel reprocessing facility progresses simultaneously with the development and demonstration activities. The commercial-plant studies and the demonstration activities interact closely to provide validity to the demonstration and verify the potential advantages of the IFR concept for commercial development.

105 ANL-WEST ENGINEERING SUPPORT GROUPS - A, B, C

Chem.
Civil Engr.
Comp. Sci.
Elec. Engr.
Envr. Sci.
Indus. Safety
Mech. Engr.
Nucl. Engr.
Radio. Chem.

The support functions of ANL-West Division include many site-wide services to EBR-II, ZPPR, TREAT, and HFEF. The following groups are of interest to students:

A. Site Engineering provides engineering design and project management support for new buildings, building additions and modifications to the physical plant facilities. (Basically an in-house architect-engineering organization). The functional engineering specialities include project, mechanical, electrical, civil, architectural and structural. Other services provided include hydrogeological assistance, environmental impact analysis, drafting, document control, photo lab, copy center, graphic arts and record management.

B. The Safety, Security and Safeguards Department is responsible for the safety, environment, security and safeguards for the ANL-W Site. Safety responsibilities include radiation protection and engineering, industrial safety, industrial hygiene and fire protection. Environment includes the control of waste, control of emissions, monitoring and sampling. Security is involved in security engineering for detection, barriers and communication and in physical control. Safeguards is responsible for the control of special nuclear material.

C. The Analytical Laboratory provides chemical analyses of both nonradioactive and radioactive materials in support of ANL-W experimental programs and facilities. The Analytical Laboratory consists of a hot cell facility for handling and performing surveillance analyses on irradiated fuels and materials; several general purpose laboratories for analyses of low-level radioactive fuel and materials; and gloveboxes for analyses of U-Pu-Zr fuel produced in the Experimental Fuels Laboratory (EFL). The Analytical Laboratory effort is primarily focused on providing both analytical and technical support to EBR-II, HFEF, and the IFR programs. Extensive chemical and radiochemical analyses are performed on a variety of samples to assure environmental safety throughout the ANL-West site.

BIOLOGICAL AND MEDICAL RESEARCH DIVISION (BIM)

Research in this division is aimed at defining the biological and medical hazards to humans from energy technologies and new energy options. Health-related studies are supported by fundamental research in a variety of scientific disciplines, including molecular and cellular biology, biophysics, genetics, radiobiology, photobiology, pharmacology, biochemistry, chemistry, epidemiology, statistics, and environmental toxicology. The research involves a convergence of various scientific disciplines with an integration of findings from investigations at the molecular, cellular, tissue, organ, and whole-animal levels, with the ultimate aim of applying these findings to problems of human health. The Division is organized into four scientific sections (Biophysics, Environmental Health, Molecular and Cellular Biology, and Radiation Biology), Each section comprises several research groups, considerable interaction occurs among all of the groups in the Division. Divisional support facilities include an editorial office, a computer center, a biomedical library, and an instrument design and maintenance shop. Opportunities for technical writing/editing internships are available in the editorial office.

BIOPHYSICS SECTION

106 ELECTRON MICROSCOPY OF MACROMOLECULAR ASSEMBLIES

Bio.

Bio-chem.

Molec. Bio.

Bio-phy.

This project focuses on the structure, function, and dynamics of assemblages of macromolecules as determined by high-resolution electron microscopy, with special emphasis on ensembles that are biologically important but are unsuitable for x-ray crystallographic analysis. Currently under study are the red cell membrane skeleton, ornithine aminotransferase, cholera toxin, amyloid fibrils, and adenovirus-associated virus. All of these biologically important macromolecules form small crystals or crystal nuclei that cannot be examined with crystallographic techniques but are suitable for electron microscopic studies. Special techniques used in this program are low-dose cryoelectron microscopy of frozen-hydrated specimens and computer-generated three-dimensional image reconstruction from two-dimensional projections obtained at various tilted angles. Major equipment includes a Philips 420, and a Jeol 100CX electron microscope located in the Materials Science Division, a Philips CM10 located in the laboratory of Dr. Josephs at the University of Chicago and a Philips 420 and Jeol 100 CX, both equipped with low-dose regulator and cryospecimen holder and located at the University of Arizona. Also available to the program are He-Ne laser-diffractometer and computer image-processing facilities at the University of Arizona.

107 MACROMOLECULAR INTERACTIONS

Bio.
Biochem.
Biophys.
Chem.

Interest in the quantitative characterization of biological macromolecular interactions was at one time effectively limited to biophysicists and physical biochemists studying the fundamental mechanisms that accounted for the specificity of these interactions. In recent years, however, interactions between biological macromolecules have become central to several areas of basic research and applied technology. For instance, interactions between antibody and antigen trigger physiological immune responses but also make possible the immunodiagnostic industry. Interactions between antibodies and chemically synthesized peptides may contribute to the development of clinically safe vaccines. Binding of short oligonucleotide probes by chromosomal DNA is used to study gene expression during cellular differentiation and transformation and will have clinical diagnostic use. Interactions between proteins and DNA form the basis of gene regulation. It is the interest of the Macromolecular Interaction group to study the expression of the kinetics and affinities of macromolecular interactions both in vivo and in vitro. As part of this effort we are developing systematic high performance liquid chromatography methods that will be suitable for use in a wide spectrum of these analyses by researchers studying the physiological role of these molecules. These methods will also contribute to the research and development of biotechnological applications of biomolecules.

108 PROTEIN CRYSTALLOGRAPHY AND INSTRUMENTATION

Bio.
Biochem.
Biophy.
Comp. Sci.
Synch. Radia.

This program uses crystallographic methods to determine the structure of proteins and their associated smaller molecules. It also seeks to advance the methods of protein crystallography by developing improved or new instruments in this field. The program operates the Midwest Area Detector Facility for Argonne and outside scientists and is developing new area detectors for laboratory and synchrotron x-ray sources. The program is now establishing two new experimental facilities for protein crystallography at Brookhaven National Laboratory's National Synchrotron Light Source (NSLS) and is developing plans for major experimental facilities in structural biology and medical imaging at the Advanced Photon Source (APS) being built now at Argonne. In addition to the NSLS facilities, this program operates two rotating-anode x-ray generators, three electronic area detectors, a molecular modelling graphics workstation, a complex computer network, and a complete modern protein chemistry laboratory. Current projects include the structure and function of diptheria toxin, cholera toxin, a steriod isomerizing enzyme, cytochrome c, and defensins.

109 PROTEIN CRYSTALLOGRAPHY AND MOLECULAR MODELING

Bio.
Biochem.
Biophy.
Comp. Sci.

The principal aims of this program are the isolation and characterization of biologically important macromolecules, the determination of their detailed three-dimensional structures in crystalline and aqueous phases, and the correlation of structure with biological function. The biomolecules under study include various antibodies and the photosynthetic reaction center. The techniques used in this program are taken from a variety of disciplines including protein chemistry, chromatography, immunochemistry, protein crystallography, computer modeling of protein structures, and computer simulating of macromolecular interactions. Major equipment includes x-ray diffractometers, a rotating anode x-ray generator with cameras, an interactive computer color graphics terminal for manipulating macromolecules in three dimensions, and computer-interfaced high-performance liquid chromatography systems.

110 PLANT BIOTECHNOLOGY

Bio.
Biochem.
Biophy.
Genetics
Molec. Bio.

This program, which studies photosynthesis, is aimed at understanding how a transmembrane protein complex, the photosynthetic reaction center, functions in the process by which light energy is converted into chemical energy. In order to understand how the three-dimensional structure of the photosynthetic reaction center defines its function, specific changes are being made in the primary amino acid sequences of reaction center proteins by site-directed mutagenesis. Several techniques of molecular biology and genetics are used to create mutations in the reaction centers from Rhodobacter capsulatus and Rhodobacter sphaeroides, two species of photosynthetic bacteria that serve as models for understanding how photosynthesis occurs in higher plants. Mutant bacteria are then screened for their ability to carry out photosynthesis, and changes in reaction center activity are determined spectrally and enzymatically. Techniques involved include DNA isolation, gene cloning with plasmid and viral vectors, gel electrophoresis, DNA-DNA hybridization, DNA sequencing, spectroscopy, and bioassay of mutant phenotypes.

ENVIRONMENTAL HEALTH SECTION

111 BIOCHEMISTRY OF METALS

Bio.
Biochem.
Chem.
Tox.

This research program is designed to investigate health effects of toxic metals to which humans may be environmentally or occupationally exposed. One research area focuses on the role of pregnancy, lactation, or ovariectomy in the susceptibility of animals to bone loss after cadmium exposure. A second area focuses on induction of the metal-binding protein, metallothionein, during midlactation. A third project evaluates exposures and responses to lead aerosols among crew members firing weapons from armored vehicles. In the first study, metals are administered orally to animals. Pathways for uptake and tissue deposition are studied with radioactive isotopes. Toxic responses are evaluated by dual photon absorptiometry; quantitative histomorphometry; analysis of calcium content and microradiographs of bone; analysis of urinary concentrations of cadmium, amino acids, proteins, glucose, and creatinine; measurements of blood concentrations of bone-related hormones, protoprophyrin, calcium, lead, and hemoglobin; and measurement of bone resorption in fetal rat limb bones in culture. Metallothionein is measured by a cadmium saturation method and identified by size exclusion and anion exchange chromatography. Major equipment available includes spectrometers for measurement of alpha, beta, and gamma emissions, an atomic absorption spectrophotometer, and high-performance liquid chromatography equipment.

112 EPIDEMIOLOGY

Bio-stat.

Epi.

The Epidemiology Group carries out studies of industrial workers occupationally exposed to radium or thorium and of persons exposed to radon gas in their homes. Cancer incidence and mortality are the major end points of interest, but morbidity and physiological end points are also considered. This research group is also studying reproductive effects in the female radium workers exposed from 1915 through the 1970s. Extensive radium body burden data are available, as are complete bone x-ray data and numerous clinical and laboratory measurements. Because of the age distribution of the female cohorts and the multigenerational nature of one population, this data base forms a resource for gerontological research. Biostatistical research on relating radiation dose to cancer risk and times of occurrence of cancer is an important aspect of this study. The thorium population is a male population, and for the residential populations from areas of high background radon concentrations, lung cancer is the primary scientific interest. Historical studies of the role of the radium dial painters upon the history of occupational medicine and radiation safety are also of interest.

113 CHRONOBIOLOGY

Behav. Sci.

Bio-chem.

Chrono-bio.

Endo-crin.

This program investigates the regulation of biological rhythms (clocks), which are affected by endogenous biological and exogenous environmental agents. Focusing on 60-Hz electromagnetic fields and carcinogenic chemical compounds as causative agents, the program integrates physiological and behavioral studies. Resulting circadian (24-h) and ultradian (< 24-h) cycles are analyzed by using a variety of standard statistical procedures and circular methods. Major equipment includes computerized data acquisition facilities for controlling environmental entraining agents and monitoring body temperature, activity, O_2 consumption, CO_2 production, animal activity, weight, and food consumption in individually housed mice and rats, as well as cell cultures. In addition, facilities for electronically describing electric fields are available.

MOLECULAR AND CELLULAR BIOLOGY SECTION

114 EFFECTS AND METABOLIC FATE OF CHEMICAL CARCINOGENS

Bio.

Bio-chem.

Chem.

This project deals with the reactions of proteins with metabolites of cancer-causing chemicals (carcinogens) that may be present in the environment or workplaces. Specifically studied are the reactions of hemoglobin with metabolites of various types of carcinogenic chemicals. Approaches and methods are being developed to analyze the products (adducts) of these reactions. The long-term goal is to analyze hemoglobin-carcinogen adducts in people to determine the degree to which they have been exposed to low levels of carcinogens and have converted the carcinogens to reactive metabolites. Many techniques typical in biochemistry and analytical chemistry are used, including purification of proteins by column chromatography, high-performance liquid chromatography, ultraviolet visible spectrophotometry, spectrofluorometry, electrophoresis, measurement of reaction rates, analysis of amino acides and peptides, and other types of chemical analyses.

115 GENE EXPRESSION IN CARCINOGENESIS

Bio.

Bio-chem.

Cell Bio.

Cell Cult.

Genetics

Carcinogenesis is considered to be a multistage process that is initiated by mutations or mutation-like events. This group studies carcinogenic processes in cultured human and rodent cells. In these cells, chemical carcinogens are analyzed for their ability to induce mutations in structural and regulatory genes. These genetic effects are related to the metabolism, tumorigenic potency, and organ specificity of the tested carcinogens. In addition, tissues collected from individuals exposed to radium (an alpha-emitter and potent human carcinogen) are tested for changes in protooncogene structure and expression. However, environmental agents may also act to promote tumor development by a nonmutational event during the postinitiation period of the carcinogenic process. Such tumor-promoting agents may affect the carcinogenic process by altering differentiation events in the susceptible cells. The project, therefore, also involves studies of the ability of tumor promoters to alter differentiation processes in various model systems, including normal and malignant human cells in culture. These processes are then related to changes in critical cellular and biochemical events, such as binding to specific receptors, changes in membrane lipid configuration, and activation and translocation of specific protein kinases or DNA topoisomerases. These studies are further extended by examining changes in the pattern of gene expression. Appropriate cDNA clones are used as probes to characterize alterations in the expression of genes coding for enzymes such as protein kinase C and inosine 5'-monophosphate dehydrogenase, which are associated with the regulation of cell growth and differentiation. Major equipment includes laminar-flow tissue-culture hoods, inverted and fluorescence microscopes, high-performance liquid chromatography equipment, protein and DNA sequence electrophoresis equipment, ultraviolet-visible light absorbance spectrophotometers, preparative and analytical centrifuges, an electronic cell counter, and a scintillation counter.

116 MOLECULAR PHOTOBIOLOGY

Bio.

Bio-chem.

Cell Bio.

Genetics

Photo-bio.

Radiobio.

This program identifies the chemical changes in the genetic material of cells caused by carcinogenic radiations, and explores the fundamental mechanisms whereby these changes are effected. Currently, emphasis is placed on DNA modifications and their effects on cells as a result of exposure to ionizing radiation or the carcinogenic solar radiations present in the environment. Procaryote and eucaryote cells in culture, as well as whole animals, are irradiated. DNA cloning and sequencing techniques are used to identify the resulting molecular changes. In addition, specific details of reactions involving nonDNA intermediates (cellular photosensitizers) and excited species of molecular oxygen are also studied. Techniques used include mutagenesis and transformation bioassays, chromatography, and analytical isopycnic and zonal ultracentrifugation, electrophoresis, and alkaline and neutral elution. Major equipment includes sources of unusually intense well-characterized ultraviolet and visible radiations of the type abundantly present in the terrestrial environment, preparative and analytical centrifuges, and scintillation counters.

117 PROTEIN MAPPING

Bio.
Biochem.
Comp. Sci.
Genetics
Immun.

This program focuses on the analysis of protein alterations that occur as a result of exposure to ionizing radiation, carcinogens, or other environmental chemicals. Two-dimensional gel electrophoresis is used to separate proteins into patterns from which data is obtained with the assistance of a computerized image analysis system. Current studies include detection of heritable mutations induced by either irradiation or treatment with toxic chemicals, analysis of altered protein expression in systems (cells or individuals) exposed to radiation or chemicals (including drugs), and biochemical characterization of the altered proteins in order to understand the mechanism by which such alterations occur. In addition to using the technique of two-dimensional electrophoresis (isoelectrofocusing followed by sodium dodecyl sulfate polyacrylamide gel electrophoresis), the group uses tissue culture techniques, including metabolic labeling with radioisotopes, and several classical biochemical techniques, including column chromatography, subcellular fractionation, and immunoblotting. For image analysis of the two-dimensional gel electrophoresis patterns, the project has a VAX 780 computer, a VAX 3200 workstation, an Eikonix scanner, two Floating Points Systems Array processors, and a GOULD IP8500 image processing system.

RADIATION BIOLOGY SECTION

118 MOLECULAR AND CELLULAR RADIOBIOLOGY

Biochem.
Cell Bio.
Genetics
Cell Cult.
Cytogene.
Molec. Bio.
Radiobio.

This program is investigating radiation-induced cellular, cytogenetic, and molecular damage that causes or contributes to the cancer induction. This information will extend our understanding of the nature of cancer induction and also lead to the development of safer limits for radiation exposure and the development of preventive/protective measures. Our approach toward understanding the carcinogenic risks associated with exposure is to examine mammalian cells for the effects of different radiation types (x-rays, gamma rays, neutrons, alpha particles, etc.) at multiple levels, i.e., gene, DNA, chromosome, and cell. In addition we look at several cell types having different characteristics, such as different abilities to repair DNA damage. In this way we hope to learn about the processes by which radiation-induced DNA lesions become mutagenic and carcinogenic. Studies have focused on how differences in DNA repair background, chromosome structure, and gene locus (sequence and genomic location) influence gene mutation induction (quantity and quality), DNA strand break induction and rejoining, chromosome aberration induction, and cell killing. Results from studies with cells in culture are compared with analysis of material from radiation-induced tumors in animals. By combining molecular, biochemical, cytogenetic and cellular assays of DNA damage induction and repair, we hope to understand the nature of the lesions produced by radiation and how they become mutagenic.

119 INTERSPECIES RADIATION PATHOLOGY

The objective of these studies is to determine the detailed lifetime response of dogs to continuous low-level radiation at a range of exposure rates from a ^{60}Co gamma-ray source. Both daily irradiation dose rate and accumulated total exposure are evaluated. The effects include life shortening, tumorigenesis, and hematological changes, including leukemogenesis. Interspecies comparisons of responses are aimed at developing rational models of radiation-induced injury that will enable extrapolations to effects in exposed populations of humans. Major equipment includes five gamma-ray rooms that can deliver brief single or continuous exposures to large or small animals (mice or dogs) at exposure rates of 0.4 R/day to 20,000 R/minute, as well as complete clinical, surgical, necropsy, diagnostic, radiographic, hematological, and histopathological facilities, and kennel space to support acute or duration-of-life studies in beagles derived from an established closed breeding colony.

Bio. *Biochem.* *Chem.* *Comp. Sci.* *Immun.* *Pathol.* *Radiobio.* *Vet. Med.*

120 MOLECULAR RADIOBIOLOGY

Molecular studies focus on the effects of low-dose neutron irradiation on the activation of specific gene sequences. This work will examine genes activated and repressed by ionizing radiation and will identify protective and repair mechanisms used by cells following exposure to irradiation. Techniques used include Northern and Southern blotting procedures, nucleic acid hybridization, cDNA cloning, DNA sequencing and transcription run-on assays. Major equipment includes all major radiation exposure facilities of the division (JANUS reactor, gamma-ray exposure rooms, and x-ray equipment).

Bio. *Biochem.* *Molecbio.*

121 RADIATION BIOLOGY AND CARCINOGENESIS

This group is concerned with the mechanisms underlying radiation mutagenesis, transformation, and carcinogenesis as they relate to the effects of low-level neutron and ^{60}Co gamma irradiation in mice. Several species of mice, are subjected to single, fractionated, or duration-of-life exposures to radiation. Life shortening, degenerative changes, incidences of specific tumor types and selected molecular end points are measured and analyzed, with emphasis on DNA damage and repair, in a variety of target tissues. Radioprotective chemicals are also used in these studies to further elucidate mechanisms of action. Data from these studies are then used in the formulation of dose response models to predict radiation hazards to man. Major equipment includes the JANUS reactor that produces fission-spectrum neutrons (0.85 MeV mean energy, only 3-4% gamma ray contribution; dose rates of 0.002-25 cGy/minute available), five gamma-ray exposure rooms that can deliver brief single or continuous exposures at exposure rates of 0.4 R/day to 20,000 R/minute, x-ray machines, an ultracentrifuge, a spectrofluorometer, an automated flow cytometer, alkaline elution fraction collectors, a phase contrast microscope, and incubators.

Bio. *Comp. Sci.* *Genetics* *Radiobio.* *Radiophy.*

122 RADIATION HEMATOLOGY

The objective of this project is to elucidate the cellular basis of radiation-induced diseases of the blood-forming tissues (i.e., aplastic anemia and leukemia). Mechanisms of damage are explored in terms of both target cell and whole tissue dysfunctions in the gamma-irradiated dog by morphological, biochemical, cytogenetic, and cell culture approaches. Major equipment includes cell culture incubators, laminar flow hoods, centrifugation and fractionation equipment, light microscopes, image analyzing equipment, and transmission and scanning electron microscopes and ancillary preparative equipment.

Biochem. *Cell Bio.* *Radiobio.* *Ultrastruc.*

CHEMICAL TECHNOLOGY DIVISION (CMT)

This Division is a multidisciplinary research and development organization in which engineers and scientists bring their diversified talents to bear on a wide variety of problems, most of which are related to the nations's energy and environmental needs. Currently, emphasis is being given to the development of near-term and advanced batteries; fossil energy utilization, primarily fluidized-bed combustion of coal and magnetohydrodynamics; recovery of energy from municipal waste; studies of reactor fuel reprocessing, geochemical studies and radioactive waste management; support for the National Breeder Reactor Research Program; magnetic fusion energy, primarily tritium recovery and dosimetry and radiation damage studies; fuel cell research and development; and environmental chemistry studies. All Chemical Technology Division projects are backed up by strong basic research. Thermodynamic studies and studies of phase relationships, molecular structure, surface chemistry, analytical chemistry, metallography, mathematical modeling, and reaction kinetics are carried out to gain a better insight and understanding of the underlying phenomena upon which major engineering projects are based.

123 ENVIRONMENTAL PROGRAM SUPPORT INTERNS

Envr. Sci.

DOE is conducting a large scale research and development program to improve its ability to clean up environmental contamination at its sites. This office provides programmatic and technical expertise and monitors about 100 R&D activities at various organizations. Interns will be assigned managment tasks and will learn about the program.

FUEL CELL R & D

124 ADVANCED FUEL CELL DEVELOPMENT (MCFC)

Ceram.
Chem.
Chem. Engr.
Metal. Engr.
Phy.

The objective of the program is to provide solutions to current technical problems identified in the DOE Molten Carbonate Fuel Cells (MCFC) Program. Research is concentrated on materials and component development for, and testing and modeling of, MCFC. Research is related to (base materials or coatings and composites) development of corrosion resistant materials and new electrode and electrolyte materials and structures. It may involve characterization of materials and components such as vapor pressure of electrolytes; electronic and/or ionic conductivity of various components; crystal defect studies (e.g., conductivity, TGA, valence state analysis); and analysis of in-cell behavior of components (e.g., sintering, migration, and phase stability, morphological and chemical stability). Modeling research is being done and involves experimental verification as well as model development and application.

125 ADVANCED FUEL CELL DEVELOPMENT (SOFC)

Ceram.
Chem.
Chem. Engr.
Metal. Engr.
Phy.

Research activities are concentrated on the development of a new, high power density fuel cell. This unique fuel cell design employs thin ceramic layer components in a strong, lightweight structure of small cells, and so achieves unequaled power per unit mass or volume. Efforts are directed toward defining materials and fabrication methodology in order to achieve the desired structure and properties for the electrolyte and electrodes. The project involves the synthesis and characterization of high temperature, inorganic materials, including x-ray, surface area, electron microscopy, and other techniques. The project also involves the fabrication and characterization of ceramic structures using tape casting, slip casting, extrusion, complex impedance measurements, and other techniques. There is a continuing effort to enhance understanding of the fundamental mechanisms of fuel cell operation and to improve fuel cell design and operation. Major equipment includes tape caster, furnaces, AC impedance system, computer, and scanning electron microscope.

NUCLEAR FUEL REPROCESSING AND NUCLEAR WASTE MANAGEMENT

126 GLASS HYDRATION STUDIES

Archeo.
Chem.
Mat. Sci.

When glass is contacted by water vapor or liquid water, alteration reactions occur. Water penetrates into the glass forming a hydration layer and displaced atoms diffuse to the glass surface and form minerals. These reactions are of interest to archaeology since hydration aging dating of natural glasses is a subject not well understood. These reactions are also important to nuclear waste management since such surface alteration will affect the waste form behavior over extended storage periods. This program investigates the kinetics and mechanisms of these reactions using surface analytical techniques such as scanning electron microscopy. Major equipment includes: scanning electron microscope, transmission electron microscope, energy dispersive X-ray analyzer, laser Raman spectrometer, Fourier transform infrared spectrometer.

127 APPLIED RESEARCH ON THE SEPARATION AND RECOVERY OF METAL IONS

Chem.
Chem. Engr.

Currently, research is being done on both the chemical and chemical engineering aspects of metal ion separation and recovery for the nuclear industry. Projects include the development of solvent extraction process flowsheets for nuclear waste management. This development will greatly reduce the costs of waste disposal and increase safety by separating radioactive elements from nonradioactive ones. The research uses radioactive tracers and computer modeling, among other methods, to simulate and evaluate potential flowsheets. A participant assisting this group would have the opportunity to learn state-of-the-art techniques in separation science and technology as well as gain practical experience in problem solving.

128 TREATMENT OF IFR WASTE SALT

Chem.
Chem. Engr.
Process Metal. Engr.

The participant will assist in studies of methods for immobilizing waste salts and metals from the IFR fuel recovery process. They will assist in setting up and conducting experiments related to the direct encapsulation of chloride salts, dispersal of salts in a ceramic or metal matrix containing zeolites, direct melting and encapsulation of metal wastes, and dispersal of the metals in a metallic matrix. They will also help in analyzing and interpreting the results of these experiments.

APPLIED ELECTROCHEMICAL RESEARCH

129 POST TEST CELL ANALYSES

Chem.
Chem. Engr.
Mat. Sci.
Metal. Engr.

The Analysis and Diagnostics Laboratory is a center for research on new and evolving battery systems. One major activity is post-test analyses of batteries and cells. These examinations determine the causes of failure, provide information on electrode performance, and identify corrosion reactions and rates. These findings are essential to the design and development of improved cells. Batteries currently under study include sodium/sulfur and lithium-alloy/metal-sulfide, two batteries with potential applications as power sources for electric vehicles and on satellites. The project calls for active participation by the participant in all phases of the examination process: disassembly, preparation of sample for physical and chemical analyses, and optical and scanning electron microscopy of air-sensitive electrode materials. Major equipment includes: metallograph, scanning electron microscope, and energy dispersive spectrometer.

130 MOLTEN-SALT ELECTROCHEMICAL ENGINEERING

Ceram. Engr. *Chem.* *Chem. Engr.* *Elec. Engr.* *Mat. Sci.* *Mech. Engr.*

The goal of this program is development of a sealed biopolar lithium/iron sulfide battery for electric vehicles and other specialized applications. A high-temperature metal/ceramic seal is being developed for compatibility with molten-salts. The research involves advanced materials, cell design, and parametric evaluation for enhancing cycle-life and performance. Cells are fabricated and tested with the aid of reference electrodes to evaluate advances in electrode or cell hardware components. Basic electrochemical data is generated to support new concepts. A demonstration battery is to be built. Major equipment includes: glovebox fabrication facility, computer-controlled test equipment, ceramic development equipment, potentiostat and programmer.

131 ELECTROCHEMICAL CHARACTERIZATION STUDIES

Chem. *Chem. Engr.* *Comp. Sci.* *Elec. Engr.*

Studies are being conducted to investigate the parameters that affect the performance of electrodes and other cell components. In these studies, attempts are made to characterize the performance of the cell component and to vary its design and composition to enhance its performance. Major equipment includes: potentiostats, galvanostats, coulometers, pulse generators, oscilloscopes, data acquisition systems, and computer controlled hardware.

132 SOLID ELECTROLYTE CELL RESEARCH

Ceram. *Ceram. Engr.* *Chem.* *Chem. Engr.*

This research effort is directed toward the development of high-performance sodium-transition-metal-chloride cells. Studies are being conducted to optimize design and chemistry of the transition-metal-chloride electrode, to develop cell components and to establish performance criteria for the cell. Major equipment includes: frequency response analyzer, differential thermal analyzer, dilatometer, optical microscopy, scanning electron microscopy, electrochemical analytical equipment, and computer-controlled data acquisition.

133 NOVEL MATERIALS FOR USE IN SOLID STATE FUEL CELLS

Ceram. *Ceram. Engr.* *Chem.*

This research effort is directed toward the development of new materials for use in a moderate-temperature range (500-800°C) fuel cell. Studies are currently being conducted to find new, highly conductive materials for use as the anodes, cathodes, electrolytes and interconnects. Effort involves synthesis of materials, sintering and processing of materials, characterization of electrochemical and chemical properties. Major equipment includes: frequency response analyzer, differential thermal analyzer, dilatometer, optical microscopy, scanning electron microscopy, electrochemical analytical equipment, and computer-controlled data acquisition and reduction.

134 URANIUM PLATING STUDIES

Chem. *Chem. Engr.* *Comp. Sci.* *Metal. Engr.*

Studies are being conducted to investigate the parameters that affect the morphology of uranium metal when it is plated from molten salt electrolytes. In these studies, attempts are being made to eliminate the formation of dendritic deposits. Parameters being investigated include plating mode (pulse, d.c. etc.), temperature and uranium concentration. The objective of these studies is to develop a process for the fabrication of uranium fission targets for the preparation of ^{99}Mo. The latter material is being used commercially for the preparation of ^{99}Tc, a radiotracer, used for clinical applications. Major equipment includes: potentiostat, coulometer, pulse generator, and oscilloscope.

HAZARDOUS WASTE AND BIOTECHNOLOGY

135 MICROWAVE ASSISTED DETOXIFICATION OF HAZARDOUS WASTE

Chem.
Chem. Engr.
Envr. Sci.

The proposed research is targeted towards developing new processes for (1) microwave-assisted detoxification of hazardous organics in waste and (2) wet catalyzed air-oxidations inclusive of heterogeneous and homogeneous catalysis. A 6 KW-microwave reactor capable of chemical/catalytic processing of waste streams is available. The current effort involves research on microwave-activated oxidation/combustion of trichloroethylene in fluid-bed over ceramic granules. Other related efforts may be directed towards developing microwave-assisted techniques for sintering of ceramic bodies or powders.

136 BIOCORROSION STUDIES

Chem.
Chem. Engr.
Elec-chem.

Studies are being initiated to investigate the rate of biocorrosion of iron specimens using electrochemical techniques. In this technique the rate of corrosion is being measured by observing the microevents in the passive oxide film covering the iron surface.

The abilities of certain bacteria to enhance corrosion have been measured by using a microorganism concentration cell. Two identical metal electrodes are placed in separate compartments that are linked via a porous frit. An appropriate electrolyte is added to the cell and one electrode compartment is then infected with a defined bacterial strain. The corrosion reaction is then monitored using classical electrochemical techniques. All metal surfaces, with the possible exception of nickel-chromium and titanium appear to be vulnerable to biocorrosion. Cold-rolled metals corrode much faster than hot rolled, and gas--welded joints corrode faster than arc-welds. Major equipment includes: EG&G corrosion measurement system.

137 RESPONSE OF SOIL MICROBES TO TOXIC CHEMICAL EXPOSURE

Bio.
Bio-chem.
Chem.
Chem. Engr.

Studies are being conducted to determine the effect of mixtures of toxic chemicals, including decontamination agents, on microbial soil populations. Previous research has shown that the responses are complex, and include enhancement as well as depression of microbial growth. Future experiments will seek to determine the mechanism of the effects, and the nature of the differences that were observed to occur among microbial species. These experiments will include the use of both natural soil samples and simulated environments. In some cases, tracer bacteria and fungi will be used to follow the fate of selected laboratory strains in treated soil. Special attention will be paid to those microbial groups that might be able to degrade and detoxify the agents. This research is also expected to provide information on chemically induced changes in the interactions between microbial species, and how these may affect the persistence of detrimental bacteria in the environment.

138 RED WATER TREATMENT PROCESS

Chem.
Chem. Engr.
Envr. Sci.

Red water is the name commonly applied to the effluent from the sellite purification treament of crude TNT. TNT is no longer produced in the United States because of environmental concerns associated with this red water waste stream. Staff members at Argonne are developing a new process for treating red water. In this process the first step is to separate the organic constituents in red water from the inorganic salts using foam fractionation, flocculation, biphasic solvent extraction, or a combination of these. The stream containing the organic fraction is then treated by a biological process to convert the organics to innocuous gases and liquid products.

Current work at Argonne involves process development and scale-up from small batch experiments to a continuous lab-scale process.

FOSSIL FUEL TECHNOLOGY

139 FEUL TEST FACILITY

Chem. Engr.

Mech. Engr.

The Fossil Energy Users Laboratory (FEUL) is a multipurpose experimental facility for the development of advanced fossil fuel technologies. It has been used to obtain design data required for the steam-bottoming components in a coal-fired, open-cycle magnetohydrodynamic (MHD) power plant. The recent MHD-related experiments have investigated (1) NO_x reaction kinetics during combustion and in the hot gas stream; (2) heat and mass transfer processes in the steam plant; and (3) formation, growth, and deposition of small particles in hot combustion gases. Other planned experiments will be to develop advanced coal combustors that produce low levels of pollutants or that can burn alternative fuels such as coal-water mixtures and low volatile chars produced during the pyrolysis or mild gasification of high volatile coals. Participants would assist engineers and scientists in setting up experiments and in interpreting the test results. Major equipment : FEUL consists of two test legs: one fired by a liquid-slurry fuel, the other by pulverized coal. Each produces about 1 kg/s of gas at temperature up to 4000°F.

140 MAGNETOHYDRODYNAMICS

Chem. Engr.

Mech. Engr.

The magnetohydrodynamics (MHD) activity focuses on the development of the technical base for open-cycle, plasma MHD power plants. Current major funded tasks are associated with the steam bottoming cycle and include investigations of the behavior of NO_x and the fouling of the convective heat transfer surfaces by seed and ash, as well as the investigation of radiant heat transfer from a potassium and particulate-laden combustion gas. Technical support is also provided to the bottoming cycle Coal-Fired Flow Facility (University of Tennessee Space Institute) by assisting in the analysis of test results on NO_x destruction and tube fouling. Other tasks are on analyses of the design issues related to the integration of the topping and bottoming cycles, the establishment of a basis for materials selection, and the regeneration of seed for recycle. The major experimental activities of the MHD program are carried out in the ANL Fossil Energy Users Laboratory (FEUL).

141 ALKALI METAL EMISSION CONTROL FOR PRESSURIZED FLUIDIZED-BED COMBUSTORS

Chem.

Chem. Engr.

Pressurized (up to ten atmospheres) fluidized-bed coal combustors are being developed to provide a highly efficient and nonpolluting system to use coal to generate power. These systems employ a gas turbine to process thermal energy from the hot high-pressure combustion gases. Unfortunately, coal usually contains an appreciable quantity of sodium and potassium which, if liberated with the high-temperature combustion gases, can lead to serious corrosion of the internal turbine parts. Granular bed sorbers, which can be used to remove gaseous alkali metal compounds from high-pressure high-temperature combustion gases, are being developed. These studies involve the chemistry and physics of the high-temperature gas-solid reactions.

142 DEPOLYMERIZATION OF COAL

Studies are being conducted to develop biocalalysts capable of breaking essential structural bonds in coal macromolecules. Experimental areas include model compound design, bioscreening techniques, cell permeability studies, affinity chromatography applications, and organic phase catalysis.

BASIC AND APPLIED RESEARCH

143 FUELS AND MATERIALS CHEMISTRY

Chem.
Chem. Engr.
Comp. Sci.

This group is engaged in a study of the behavior of selected materials in environments simulating that of fission and fusion energy systems. This program is designed to provide basic data for understanding the underlying thermodynamic and kinetic constraints that serve to dictate materials stability. Opportunities exist for high-temperature thermochemical/thermophysical property studies and studies of species transport under chemical gradients as well as temperature gradient conditions. The sophisticated microanalytical techniques of electron probe microanalysis and ion microprobe mass analysis, as well as ESCA/AUGER analysis, will be applied to this research.

144 HIGH-TEMPERATURE THERMOPHYSICAL PROPERTIES

Chem.
Chem. Engr.
Mech. Engr.
Phy.

Analysis of the behavior of nuclear reactor fuel requires knowledge of thermodynamic and transport properties. These studies which include experimental and theoretical research are designed to provide the data needed for evaluation of fuel performance. Activities include differential thermal analysis and thermogravimetry studies, measurements of thermal expansion and thermal conductivity, and phase diagram calculations. Studies related to fuel-cladding interactions are also performed.

145 INTERFACIAL MATERIALS CHEMISTRY

Chem.
Chem. Engr.
Phy.

In this program advanced spectroscopic techniques (infrared, electronic absorption, nuclear magnetic resonance, Raman spectroscopy) are used to investigate the catalytic and structural properties of molecular sieve materials. The emphasis of the research is directed mainly at the mechanisms of catalysis that lead to carbon-carbon bond formation, isomerization, dehydrogenation, alkylation, and carbon-hydrogen bond activation. Aluminophosphate molecular sieves with intermediate pore sizes are a primary focal point in this effort. Major equipment used: Raman, visible, infrared and NMR spectrometers, scanning Auger/XPS instrument; scanning electron microscope with x-ray analyzer; gas chromatographs.

146 SPECTROSCOPIC AND ELECTROCHEMICAL STUDIES IN SURFACE AND INTERFACIAL CHEMISTRY

Chem.
Chem. Engr.
Elec. Engr.
Envr. Sci.
Mech. Engr.
Metal. Engr.
Nucl. Engr. *Phy.* *Mat. Sci.* *Corr. Sci.*

Areas of research are: (1) spectroscopic investigations of electrochemical systems, as well as fundamental studies of electrochemical systems, as well as fundamental studies of the structure of the solid-liquid interface and the nature of the adsorbed state; (2) corrosion and passivation behavior of metals and alloys in various solution environments and as a function of temperature; (3) measurement of charge and mass transport processes in surface films and correlation with electronic structure; (4) catalysis of electrochemical reactions by transition metal macrocyclic compounds and oxides; (5) quantum theoretical calculations of surface and double-layer structure, the solvation of ions in solution, and theory of charge transfer at the solid-solution interface. Electrochemical techniques (e.g., steady-state polarization, cyclic voltammetry, potentiostatic and galvanostatic transients, rotating ring-disc electrode, AC impedance) and spectroscopic methods (e.g., UV-visible, laser Raman, IR, and synchrotron radiation techniques) are employed in the investigations. Major equipment includes: complete electrochemical instrumentation; laser Raman, UV-visible, IR spectrometers; high temperature-high pressure aqueous corrosion facility.

147 FLUID CATALYSIS

Chem.
Chem. Engr.
Phy.

Homogeneous and heterogeneous catalysis chemistry and mechanisms associated with the activation of dihydrogen, carbon dioxide, carbon monoxide and dinitrogen are explored using in-situ spectroscopic and kinetic techniques. Parallel synthetic efforts are directed toward the isolation or synthesis of organometallic reaction intermediates and new catalytic species. Catalytic C-H bond activation chemistry, catalytic formation of pre-ceramic organometallic polymers, and shape-selective macrocyclic catalysts are also investigated. Major equipment includes: high pressure multinuclear NMR facility, high-pressure FT-IR, liquid and gas chromatographs, and high-pressure autoclaves.

148 COMPUTER MODELING OF ELECTROCHEMICAL REACTIONS

Chem.
Chem. Engr.
Comp. Sci.
Math.
Phy.

Numerical simulations of electrode reactions will be carried out, incorporating the heterogeneous charge transfer reaction, homogeneous chemical reactions, diffusion to and from reaction sites, adsorption effects, and electrical double-layer effects. The nonlinear partial differential equations describing the system will be solved by numerical techniques to give the current/potential/time relation of the system after a perturbation from equilibrium. The purpose of the calculations is to extend the range of electrochemical kinetic and corrosion measurement techniques into areas which are presently inaccessible because of mathematical difficulties and to evaluate the efforts of some present techniques which use approximations to simplify the mathematics. Major equipment includes: VAX-6220 Computer, IBM Mainframe Computers.

149 ELECTROCHEMICAL KINETICS RESEARCH

Chem.
Chem. Engr.
Phy.

Kinetics and mechanism of fast electrode reactions will be investigated using microsecond-range transient techniques. The kinetics of the elementary charge-transfer step and its variation with temperature are under investigation. The kinetic data will serve as a basis for selection of the atomic mechanism of corrosion. Under investigation are the effects of minor constituents of the environment on electrochemical reaction kinetics. This effect has fundamental scientific importance, in addition to the obvious practical implications. Major equipment includes: pulse generators; Digital Storage Recorder, VAX 6220 Computer.

150 METAL MOLTEN SALT SOLUTIONS

Chem.
Chem. Engr.
Metal. Engr. *Phy.*

The behavior of metal molten salt solutions is challenging since no present theory can explain completely the chemical trends observed as the metal is changed from cesium to lithium. Electromotive force measurements are used to study the activity of the metal dissolved in its molten salt in very dilute solutions. The results will give insights into the structure of such solutions and the state of the electrons.

151 IONIC ALLOYS

Chem.
Chem. Engr.
Metal Engr.
Phy.

A fundamental study on the properties of the unusual class of alloys referred to as ionic alloys is currently underway using a variety of experimental techniques. The project will involve electrical resistivity, electromotive force measurements, and vapor-pressure measurements on Rb-Au and Cs-Au alloys. The results should give significant insights into the structure of the alloys, which are metallic at most compositions but behave as ionic systems at a 1:1 stoichiometry.

152 OXYGEN STOICHIOMETRY, STRUCTURE TRANSITIONS, AND THERMODYNAMIC BEHAVIOR OF HIGH T_c SUPERCONDUCTOR SYSTEMS

Ceram.
Chem.
Chem. Engr.

Research involves measuring equilibrium oxygen partial pressures above nonstoichiometries 1-2-3 and related systems at various temperatures by means of EMF techniques; and the subsequent calculation of pertinent thermodynamic quantities.

153 CHEMICAL EQUILIBRIUM PROGRAM

Chem.

An advanced computer program based on geometric programming is being developed for the calculation of chemical equilibria in complex multicomponent multiphase systems. The participant will help to modify and test the capabilities of the program on real problems concerning corrosion, the origins of meteorites and pyrometallurgy.

154 QUANTUM MECHANICAL STUDIES OF REACTIONS IN MOLTEN SALTS

Chem.
Comp. Sci.
Phy.

The studies involve applications of quantum-mechanical theory to reactions and reaction species in molten salts which are of fundamental scientific interest as well as of importance technologically. Large scale computations employing ab initio molecular orbital methods are being carried out to determine the energetics, equilibrium structures, and vibrational frequencies of species which exist in molten salts.

155 THEORETICAL STUDIES OF SOLVATION

Chem.
Comp. Sci.
Phy.

The solvation of anions, cations, and nonpolar solutes in aqueous solutions is being studied by theoretical methods. Investigations are being carried out on the size and structure of the first solvation shell and the effects of hydrogen bonding.

156 THEORETICAL STUDIES OF MOLECULE-SURFACE INTERACTIONS

Chem.
Comp. Sci.
Phy.

Ab initio molecular orbital methods are being used to study molecule-surface interactions. The surfaces are represented by clusters of metal atoms and molecules are placed on the surface. Binding sites, vibrational frequencies and structures are being studied. These studies are important to understanding reactions occurring in catalysis and aqueous corrosion.

157 EVOLUTION OF NATURAL HYDROTHERMAL SYSTEMS

Chem.
Envr. Sci.
Geo.
Hydro.

The objective of this program is to achieve a deeper basic understanding of the evolution of natural hydrothermal systems. Current emphasis is on chemical and isotopic studies of active hydrothermal systems at Yellowstone, Valles, Long Valley, and volcanos in the northern Andes, and fossil hydrothermal systems in the Sierra Nevada. Major equipment used: optical and electron microscopes, x-ray diffractometers, fluid inclusion microthermometry stage, alpha spectrometers, thermal ionization mass spectrometer, computer programs for geochemical modeling.

158 CHEMISTRY OF SUPERCONDUCTING CERAMICS

Ceram.
Ceram. Engr.
Chem.
Chem. Engr.

This research is directed toward the development of alternative processing methods leading to the production of high-quality superconducting ceramics in the Y-Ba-Cu-O system. The inorganic chemistry affecting the extent and modes of reaction between the metal oxides will be investigated. Major equipment includes: optical and scanning electron microscopy, and differential thermal analysis.

159 FUSION REACTOR RESEARCH

Chem.
Chem. Engr.
Metal. Engr.
Nucl. Engr.
Phy.

A variety of projects covering the chemical and engineering aspects of fusion reactor technology are available. These projects include measurement of the thermodynamic and thermophysical properties of lithium-containing metals and ceramics, the transport and release characteristics of tritium from breeder blankets, thermal response behavior for ceramic breeders, and development of neutron dosimetry and damage analysis methodology. The general aim of these projects is to develop an understanding of the behavior of breeder materials and tritium-handling requirements for fusion power reactors.

160 TRITIUM AND BLANKET RESEARCH FOR FUSION REACTORS

Chem.
Chem. Engr.
Envr. Sci.
Comp. Sci.

The aim of this program is to develop tritium-handling and chemical processing technology applicable to tritium systems for fusion reactors and for heavy water fission reactors. Projects include engineering design and parametric (computer) analysis of tritium systems. Current programs focus on integrating a tritium processing system for a fusion blanket into the experimental tritium fuel cycle at Los Alamos. Major equipment: Liquid scintillation counter.

161 DEEP CARBON GEOCHEMISTRY

Chem.
Geo.

The objective of this program is to define the limiting geological conditions under which hydrocarbons may be generated or transported. The current focus of the work is on the thermal and chemical interactions between magmatic intrusions and hydrocarbon-bearing rocks in sedimentary basins (e.g., Animikie Basin (MN), Culpepper Basin (VA), and Durham Basin (NC). Major equipment includes: optical and electron microscopes, fluid-inclusion microthermometry stage, high vacuum gas separation lines, gas chromatograph, mass spectrometers.

ANALYTICAL AND ENVIRONMENTAL CHEMISTRY

162 TRACE ORGANIC ANALYSIS OF ENERGY AND ENVIRONMENTALLY-DERIVED MATERIALS

Chem.
Comp. Sci.
Envr. Sci.

A wide variety of chemical carcinogens and toxins with potential health and safety implications are analyzed. Chemicals responsible for hazards are identified and measured. Methods used include gas chromatography (GC), combined gas chromatography/mass spectrometry (GC/MS), high-performance liquid chromatography (HPLC), supercritical fluid chromatography (SFC), Fourier transform infrared spectrometer (FTIR), wet chemistry, and computer analysis. In some cases, chemicals present below the parts-per-billion level are detected. Sophisticated computer-controlled analytical equipment is used. Major equipment includes: GC, SFC, HPLC, MS, MS/MS, and FTIR.

163 METHOD DEVELOPMENT IN TRACE-ORGANIC ANALYSIS

A variety of analytical problems are encountered for which methods are not currently available. Methods are developed to meet these needs. Recent and on-going method development examples include PCBs, dioxins, air sampling, and stack gas monitoring. Recent instrumentation development includes GC/matrix-isolation Fourier transform infrared spectrometry, multi-dimensional GC, capillary GC, and mass spectrometry. Major equipment includes: GC, SFC, HPLC, MS, MS/MS and FTIR.

164 DETECTION OF CHEMICAL AGENTS IN THE ENVIRONMENT USING ACTIVE AND REMOTE INFRARED SPECTROSCOPY

Chem.
Envr. Sci.

Environmental pollutants need to be identified rapidly for the characterization of Hazardous Waste Sites. This program develops new methodology for characterization of pollutants in gas streams and soils using Fourier Transform Infrared Spectroscopy. The techniques are also applicable for chemical warfare agent detection. Field work may be required. Major equipment includes: Nicolet 60 SX FTIR, XM21 remote FTIR, IBM compatible computers.

165 MODERN INSTRUMENTAL METHODS FOR TRACE ELEMENT ANALYSIS

Modern instrumental techniques are being used to characterize trace inorganic elements in a broad range of sample matrices. Elements of environmental and technical importance are being studied. Activities include the development of improved methods of sample preparation and analysis. Instrumentation available includes: atomic absorption spectrophotometers (both flame and flameless), inductively coupled plasma-atomic emission spectrometer, ion chromatograph, X-ray fluorescence spectrometer, and laser fluorescence uranium analyzer.

166 DETERMINATION OF OXYGEN IN LOW-MELTING METAL ALLOYS

Chem.

Combustion and inert gas fusion methods are being applied for the determination of hydrogen, oxygen, and nitrogen in metals. The method has been demonstrated to be sensitive to microgram amounts of these gases in metals which possess high melting points. However, variable results for the determination of oxygen have been obtained for metals with relatively low melting points, i.e., Pb, Mg, and Cd. The success of the method depends upon several physical and chemical phenomena associated with the metal or alloy of interest. The study of these phenomena and their elucidation provides an interesting and challenging project.

CHEMISTRY DIVISION (CHM)

The areas of investigation in this Division include chemical science, materials science, and nuclear medicine research. Chemical sciences research covers such areas as radiation chemistry, photosynthesis, theoretical chemistry, metal cluster chemistry, intramolecular dynamics and chemical kinetics, separation chemistry, coal chemistry, inorganic fluorine chemistry, and chemistry of the actinide elements. In materials science the research concerns the chemistry of surfaces and interfaces, the preparation and characterization of organic conductors and superconductors, and structural studies of materials important to energy technologies.

167 RADIATION CHEMISTRY AND PHOTOCHEMISTRY

Bio.
Chem.
Phy.

Chemistry induced by ionizing radiation is studied utilizing state-of-the-art accelerators and lasers. The identity and dynamics of transient intermediates produced by pulse radiolysis or laser photoionization are examined to learn about the mechanisms of energy deposition, transformation and transport in condensed media. Current studies include experimental and theoretical studies of electron solvation and reactivity, radical cation transformations and reactions in condensed phase, studies of H atoms, charge-pair dynamics and excited states in photoionization and radiolysis. New ventures include radical cation chemistry of highly strained molecules, ion-molecule reactions in condensed phase, new matrix isolation methods, and use of noble gas solvents.

These studies have broad relevance to many fundamental problems in chemical reactivity, to radiation-induced polymer modification, and to the understanding of biological effects of ionizing radiation. Appropriate techniques are used to study real-time behavior of transient species. Picosecond absorption and emission studies are carried out with pulse-probe, streak camera, and photon-counting methods. Studies in the nanosecond time domain include DC-conductivity, optical and special time-domain magnetic resonance methods.

168 BASIC RESEARCH ON SOLAR ENERGY CONVERSION

Chem.
Phy.

The combination of radiation and photochemical techniques is utilized to study basic problems relevant to the field of solar energy conversion to useful fuels or chemicals. Photochemistry in semi-organized environments (e.g. micelles, polyelectrolytes, vesicles, etc.) is studied to determine the factors governing electron transfer from excited dye molecules to a variety of acceptors as well as the dark back electron transfer reactions. Mechanisms of the catalysis needed in such conversion systems are investigated under active catalytic conditions during illuminations. The catalysts used are usually colloids of metals, semiconductors or a mixture of both.

169 ELECTRON TUNNELING BETWEEN MOLECULES

Chem.
Phy.

Quantum mechanical tunneling transfers electrons up to 35 angstroms between molecules trapped in rigid matrices. We use gamma irradiation, a pulsed electron beam or pulsed lasers to create ionization. The long-range electron-transfer processes and the spectroscopy of the ions are studied by their characteristic light absorption and/or emission. Understanding the chemical physics of these processes may lead to applications in photosynthesis and photochemical solar energy storage.

170 CHLOROPHYLL FUNCTION IN PHOTOSYNTHESIS

Chem.

Bio. chem.

Research includes: Chemistry of chlorophyll and bacteriochlorophyll; isolation and characterization of photosynthetic pigments, enzyme synthesis of chlorophyll model systems for studies of artificial photosynthesis; chlorophyll-protein interactions and models of chlorophyll-antenna protein complexes; application of mass spectroscopy and small angle neutron scattering to the composition and structure of chlorophyll aggregates.

171 PHOTOSYNTHESIS: THE PRIMARY EVENTS AND ASSOCIATED MOLECULAR STRUCTURES

Biochem.

Chem.

The photosynthesis research begins with the large scale growth of photosynthetic organisms (algae and bacteria) and extends to experimental and theoretical investigations of the first few billionths of a second of photosynthesis. These investigations emphasize the femtosecond kinetics and associated molecular structures involved in the initial light-induced chemical reactions of photosynthesis. Single crystals of photosynthetic proteins are probed by advanced spectroscopic techniques, including electron spin resonance, electron spin echo, nuclear magnetic resonance, time-resolved optical spectroscopy, time-resolved optically detected magnetic resonance and mass spectroscopy. All experiments are under computer control. Fundamental interpretation of the experimental results utilizes theoretical modeling of photosynthesis and/or magnetic resonance that is conducted with a large variety of computers.

172 BIOMIMETIC APPROACHES TO SOLAR ENERGY CONVERSION: ARTIFICIAL PHOTOSYNTHESIS

Biochem.

Biophy.

Chem.

The artificial-photosynthesis program is designed to mimic the primary events of photosynthesis. The approach involves the preparation of modified chlorophylls and other model compounds so constructed as to reproduce key features of the initial charge separation act of photosynthesis. The research includes the incorporation of synthetic photoredox molecules in proteins and membranes. The photoactivity of the artificial models is probed by advanced computer-controlled spectroscopic techniques, including NMR, femtosecond optical absorption, time resolved optically detected magnetic resonance, electron-spin resonance and electron-spin echo. Emphasis of interpretation is placed on the mechanism and kinetics of biomimetic redox reactions.

173 CHARACTERIZATION OF MACROMOLECULES BY MASS SPECTROMETRIC TECHNIQUES

Chem.

The objective of this study is to characterize large molecules derived from fossil materials such as coals and kerogens and from biomacromolecules. Soft ionization techniques such as low voltage electron impact and fast atom bombardment create the ions, followed by high resolution mass spectrometry and tandem mass spectrometry to identify the ions formed. Other approaches used include pyrolysis (Py) gas chromatography-mass spectrometry and Py-microwave induced plasma spectroscopy. Projects vary from instrument development to applications in energy research.

174 SYNTHESIS AND CHARACTERIZATION OF NOVEL ORGANOMETALLIC PRECURSORS TO HETEROGENEOUS CATALYSTS

Chem. The focus of the synthesis program is to explore and to develop new chemistry that will allow the preparation of a new generation of heterogeneous catalysts. The new chemistry will be directed toward the development of catalytic systems having the desired size and shape selectivity, catalytic activity, and low susceptibility to poisoning for upgrading low-quality hydrocarbon sources to fuels and chemicals. The approach involves the synthesis of large, multi-dimensional organometallic templates as precursors to metal oxide catalysts. A second aspect of the research involves solution and solid phase spectroscopic investigations to characterize precursors and products, computer modelling to and in the design of new precursors, and correlation of the information to gain insight into the chemical and physical interactions important in catalyst formation.

175 CATALYSIS: SYNTHESIS OF NEW MATERIALS

Chem. Two current national concerns are the development of cleaner energy sources and the extension of our own energy reserves. Both of these issues can be addressed by research into new catalysts. The specific project in our group involves the synthesis and characterization of new catalysts that are designed to be used for hydrocarbon processing by the oil industry. The nature of this work combines aspects of inorganic chemistry, geochemistry and physical chemistry. Experiments involve bench-scale preparation of these inorganic catalysts using inorganic solid-state techniques. The silicates and other oxides are prepared from aqueous solutions treated at high temperature and pressure. Characterization is accomplished by thermal analysis methods, x-ray powder diffraction and UV-visible spectroscopy - all of which are computer-controlled.

176 COAL GEOCHEMISTRY

Geo. chem.

Org. Chem.

Understanding the processes by which organic materials are transformed, under geologic conditions, into coal and oil, ultimately helps us to better understand the structure, and hence the reactivity of these materials. In this program we are studying geochemical transformations in a number of natural plant biopolymers, which are relevant to coal structure. Both the modern biopolymers (e.g.; lignin, sporopollenin, and plant resins), and their coalified products (vitrinite, sporinite, and amber), are being isolated and characterized using a wide variety of organic chemical procedures and instrumental analyses (e.g.; GC-MS, High Resolution-MS, MS-MS, FTIR, and solid and liquid NMR). This project offers the opportunity to acquire and apply practical knowledge of organic chemistry to the characterization of a variety of modern and coalified natural products.

177 THE PREMIUM COAL SAMPLE PROGRAM

Chem.

Phy.

This program provides high-quality, well-characterized coal samples for basic coal research. Samples are sent upon order to research laboratories around the world. A Users Handbook is continually updated with new analytical information and bibliographic references. A Quarterly Newsletter is also prepared with current information of interest to users about the samples. Each document is sent to all recipients of the samples.

178 SEPARATION AND CHARACTERIZATION OF COAL MACERALS

Chem.
Phy.

Coal macerals are coalified ancient plant remains that make up the organic portion of coal and can still be microscopically identified. This program is concerned with the study of the separation and characterization of the macerals to provide more selective feed-stocks for various processes. The project is basic-research oriented and involves some methods of separation similar to those used to separate cells and cellular components. A variety of methods is used to characterize the macerals including density gradient analysis, microscopic analysis, Fourier transform infrared spectroscopy, swelling properties, elemental analysis, and molecular affinity.

179 THE CHEMICAL CONSTITUTION OF A LOW-VOLATILE BITUMINOUS COAL

Chem.
Phy.

It is our postulate that higher-ranking bituminous coals, such as the Pocahontas No. 3 coal in the Premium Coal Sample Program, have chemical compositions that are significantly less complex than the compositions of the lower-ranking oxygen-rich bituminous coals that have received so much attention. We are, consequently, working toward the discovery of new chemical and spectroscopic methods that will establish the constitution of this coal. We are focusing on solid-state ^{13}C NMR spectroscopy, high-pressure liquid-chromatographic techniques, and new strategies for the solubilization and separation of complex mixtures

180 STUDY OF POWERFUL OXIDANTS

Chem.

This research is concerned with the reactions of such compounds as fluorine, hypofluorous acid, oxygen difluoride, perbromic acid and xenon trioxide with inorganic and organic reducing agents. We are studying both the mechanisms of such reactions and the nature of new products formed.

181 THEORETICAL CHEMISTRY

Chem.
Comp. Sci.

The theoretical chemistry program includes studies of the energetics and dynamics of chemical reactions, the nonlinear dynamics of intramolecular energy transfer and the structure and spectra of molecules. Current research areas include studies of elementary chemical reactions involved in the oxidation of hydrocarbon species. This area involves the use of large-scale computers with emphasis on parallel computing.

Math. Phy.

182 EXPERIMENTAL METAL CLUSTER CHEMISTRY

Chem.
Phy.

The chemical and physical properties of clusters of metal atoms, such as Fe, Co, Ni, Cu, Al, Cr, V, and Nb, are under study. Chemical reactions are carried out in a laser-vaporization cluster source coupled to a continuous flow reactor and followed by laser ionization time-of-flight mass spectroscopy to determine product compositions. Studies of reaction kinetics, thermodynamics, catalysis, and cluster structure are being pursued. Physical properties are measured by photoionization, collisional ionization, two-photon resonantly-enhanced ionization spectroscopy, and laser-induced fluorescence. Major equipment includes: two molecular-beam machines, excimer, dye and YAG lasers.

183 THEORETICAL STUDIES OF CLUSTERS

Theor. Chem.
Phy.
Math.

Theoretical studies of chemical and physical properties of atomic clusters are carried out. These include investigation of structural and dynamical features of clusters such as geometries, isomerization and phase-charge transitions, chemical reactivity, etc. Both analytical and numerical (computer) simulation techniques are used. The work involves development of new fundamental concepts and theoretical techniques specifically tailored for applications to finite systems.

Comp. Sci.

184 STATE-TO-STATE DYNAMICS

Chem.
Phy.

This program involves the study of state-to-state inelastic or reactive processes of small radicals in a crossed beam device. Pulse-valves are used to create the two beams, laser-induced photodissociation is used to create the radicals, the crossing-angle of the two beams is used to control the relative collisional energy, and laser-induced fluorescence is used to detect the products. Current research areas focus on chemical reactions involved in the oxidation of hydrocarbon species.

185 CHEMICAL KINETICS

Chem.
Phy.

This program involves the study of reactive processes of small radicals in shock tubes. Two different shock tubes are in operation or development. In one, flash photolysis or excimer-laser photolysis is used to create radicals in the shock-heated gas mixture and the decay or formation of the atomic products is followed by atomic resonance absorption spectroscopy. In the other, the concentration of radicals in high-temperature gases immediately behind the shock front is detected by a pulse of tunable, vacuum-ultraviolet laser light created by nonlinear four-wave mixing in mecury vapor. Current research areas for both shock tube studies focus on chemical reactions involved in the oxidation of hydrocarbon species.

186 PHOTOIONIZATION-PHOTOELECTRON RESEARCH

Chem.
Phy.

A state-of-the-art high-resolution photoionization mass spectrometer is adapted to the study of atoms and molecules. The species may be normally volatile, or may be generated by high temperature, electric discharges, chemical reaction processes, or laser photodissociation. Energy thresholds and resonances in the vacuum ultraviolet are probed.

Recent experiments on open-shell atoms produced by these methods have provided unique tests of many-body theory of autoionization. A number of important transient species, which are intermediates in chemical reactions, have recently been studied. These include COOH, B_2H_5 and B_2H_4, species not previously detected in the gas phase. The results have provided information about exotic borohydride structures, and resolved outstanding questions concerning bond energies, geometrical structures, and excited state energies. A new coincidence scheme has been developed for performing photoelectron spectroscopic studies on these transient species.

187 MOLECULAR ION-LASER INTERACTIONS

Chem.
Phy.

Molecular ions from an ion source are mass selected and crossed with an ultraviolet laser beam. If photodissociation occurs, the fragment ions are detected by another mass spectrometer, which can also determine the recoil velocity in the dissociation process. With polarized laser radiation, a recent addition, the symmetry of the excited state can be inferred. This technique provides a tool for direct spectroscopic measurements on molecular ions and the energy distribution in the dissociation process. It has been utilized recently to distinguish isomeric molecular ions.

188 NUCLEAR MEDICINE

Bio.
Bio-chem.
Chem.

The nuclear-medicine research program is focused on the development of radioactive drugs for both diagnostic and therapeutic uses. This project includes the production of radionuclides, their incorporation into radiopharmaceuticals, and the testing of these compounds in cell culture and in animals. Our diagnostic studies focus on the development of synthetic neurotransmitters and neuroleptic drugs for studies of brain function, the development of agents to bind to steroid receptors in gynecologic cancers, and new heart-imaging agents.

Among the therapeutic applications that we have been investigating are the production and use of alpha emitters linked to a variety of agents for suppression of the immune system for organ transplant; the use of alpha and beta emitters linked to a variety of agents for the treatment of cancer; the production and use of low-energy electron emitters linked to steroid-receptor binding drugs for therapy; and the modification of the effect on target tissue and normal tissue by the use of radiosensitizers and radioprotectors, respectively. These studies are done in collaboration with groups in the ANL Biology Division and with hospitals and medical schools around the country.

189 X-RAY STRUCTURAL STUDIES

Chem.
Comp. Sci.
Phy.

The molecular structure of compounds with unusual solid state or chemical properties is determined by x-ray diffraction using computer-controlled diffractometers. Our interests include one-dimensional and organic conducting salts and molecules which model catalytic surface or homogeneous intermediates. Phase transitions in crystalline materials are studied using an x-ray instrument in which the sample temperature is varied from 10 to 300°K. The preparation of new materials requires a variety of techniques, including electrolytic synthesis and the manipulation of air-sensitive compounds.

190 SINGLE CRYSTAL TIME-OF-FLIGHT NEUTRON DIFFRACTION

Chem.
Comp. Sci.
Phy.

The crystal, molecular and magnetic structures of a variety of materials are studied using the single crystal neutron diffractometer at the Intense Pulsed Neutron Source. Data analysis and graphics display software are being applied to metal-hydrides, unusual organometallic compounds, and superconducting materials to obtain structure-property relationships. Structural and magnetic phase transitions are investigated at high and low temperatures and under applied pressures. The texture of polycrystalline high temperature superconducting samples is analyzed.

191 NOVEL ORGANIC CONDUCTORS AND SUPERCONDUCTORS

Chem.
Comp. Sci.
Phy.

New organic conductors and superconductors (first discovered in 1979), which have novel electrical and magnetic properties, are synthesized and then characterized using various techniques. The organic donor molecules are prepared in our laboratories and the conducting salts are grown using simple electrocrystallization techniques. Projects in this area of research include: organic synthesis; crystal growth using a variety of techniques; compound characterization using chemical analysis, IR and NMR; structural characterization using x-ray and neutron diffraction and computer analysis of results; electrical conductivity and superconductivity measurements; variable temperature electron spin resonance spectroscopy; and magnetic properties studies.

192 SURFACE AND INTERFACIAL CHEMISTRY

Chem.
Mat. Sci.
Metal Engr.
Phy.

The detection sensitivity of adsorbed species may be increased by several orders of magnitude by making use of laser ionization of neutral atoms and molecules emitted from surfaces by ion, electron- or photon-stimulated desorption. The rationale underlying the effort is that for most systems the desorbed neutral/ion ratios are very large, typically 10^3-10^5, and that laser ionization in contradistinction to other ionization methods can approach 100% efficiency. Recent advances in instrumentation take advantage of sophisticated developments in angle and energy refocusing time-of-flight mass spectrometic detection, advanced electronic pulsing and timing circuitry, and extensive computer control of instrument operation so that useful yields for sputtered atoms near 10% of the sputtered flux can now be obtained.

Future directions include extensive studies of the sputtering yield behavior of a variety of materials in the low damage regime; exploiting the element-specific nature of resonance multiphoton ionization to solve problems in geochemistry where isobaric interferences play havoc with, for example, the Ru-Os chronometer; measuring for the first time electron- and photon-induced neutral desorption yields; elucidating the mechanism of optical damage in materials, by bringing to bear our ultrasensitive detection methods at very low bombarding laser fluxes and fluences.

Surface segregation in dilute alloys (e.g., Cu-Li) is being studied under ion bombardment conditions by a variety of surface spectroscopies (Auger, x-ray photoemission, UV photoemission, ion scattering and secondary ion mass spectroscopy). The purpose is to understand processes which make it possible to produce materials in which the surface properties are significantly different from those of the bulk, and to apply the techniques developed to limiter and first-wall problems in magnetic-confinement fusion devices.

193 APPLICATION OF LIQUID-LIQUID EXTRACTION TO METALS SEPARATION PROBLEMS

Chem.

Liquid-liquid extraction systems developed in our basic studies are applied to the partitioning of the long-lived hazardous components of reactor spent-fuel process waste and to the recovery of metals of critical and strategic importance. The applications involve tracer-level and spectroscopic studies using synthetic solutions. Primary emphasis is given to the extraction of plutonium, americium, and curium and to the extraction of cobalt, nickel, and copper. These problems require evaluation of a variety of extraction systems as to their extracting efficiency, physical behavior, and behavior toward interfering ions and to the ease of recovery of extracted metals from the extractant phase.

194 PREPARATION OF ORGANIC EXTRACTANTS FOR METAL VALUE RECOVERY

The synthesis of novel organic extractants, especially organophosphorus compounds involve the utilization of literature synthetic methodology as well as the often necessary development of novel technology. Purification by a wide variety of techniques are employed, especially chromatography. Standard spectroscopic instrumentation (NMR, IR, MS) is used for identification.

195 PARTICLE-INDUCED DESORPTION/IONIZATION MASS SPECTROMETRY

Chem. *Comp. Sci.* *Phy.*

Mass spectrometry of organic molecules and biomolecules is explored using digital computer-aided time-of-flight mass spectrometry with fission fragments from ^{252}Cf, MeV energy-pulsed ion beams from the accelerators at Argonne, and laser pulses. This method has analogs in FAB, ^{252}Cf-PDMS, and Secondary-Ion Mass Spectrometry. Particle-induced desorption/ionization is used to analyze very high molecular weight compounds (>5000 amu) that are important to biochemical processes. Further studies of the particle-induced desorption process are being undertaken to provide insight into the mechanisms of energy deposition and ion desorption. Understanding the physics of this process may lead to mass analyses of entire protein complexes and DNA from organisms.

PHYSICS AND CHEMISTRY OF HEAVY ELEMENTS

This section is concerned primarily with the chemistry of lanthanide and actinide elements.

196 SOLUTION CHEMISTRY OF ACTINIDE ELEMENTS

Chem. *Radiochem.*

The reactions of actinide ions in solution are studied to provide the necessary thermodynamic and dynamic information for the development of reaction theory, environmental models, separation procedures, and nuclear medicine applications. Preparation of the reagents requires inorganic, electrochemical, and radiochemical procedures, ion exchange, solvent extraction, and analysis by spectrophotometric and potentiometric techniques. The half-lives of reactions currently being investigated may range from hours through milliseconds (stopped-flow techniques) down to nanoseconds for reactions with OH radicals and the hydrated electron generated at the Argonne Linear Electron accelerator. Participation in the kinetic studies affords the opportunity to become familiar with the use of on-line computer facilities for the stopped-flow and pulse radiolysis experiments.

197 INORGANIC-PHYSICAL CHEMISTRY OF THE ACTINIDES AND LANTHANIDES

Chem. *Radiochem.*

The 4f and 5f elements have unique and novel bonding properties. The objective of this program is to understand and to predict the structure and reactivity of compounds of the rare-earth and actinide elements. We study their oxides and halides in unusual oxidation states to characterize unusual species that are important in nuclear fuel and waste isolation technologies. We synthesize new inorganic complexes to interpret the effects of the large ionic size and 5f orbitals of actinide ions in bonding. These efforts require modern instrumental techniques: high-vacuum, fluorine, and inert-atmosphere syntheses; microchemical and radiochemical operations; x-ray diffraction apparatus for crystal structure determinations; calorimetry and electrochemistry to determine the energetics of reactions; and a wide variety of spectrophotometric techniques. Ours is one of the few laboratories in the world that studies the chemical and physical properties of transuranium elements (neptunium through einsteinium) on the milligram and microgram scales.

198 SOLID-STATE ACTINIDE CHEMISTRY

Chem.

Mat. Sci.

Systematic studies which focus on the cooperative interactions of f electrons in solids are the theme of this research effort. A program involving the determination of magnetic and superconducting properties of ceramic oxides, and how these properties are influenced by structure, is now well established. This topic has received considerable publicity since superconductivity was observed to occur at 90°K in a subclass of these oxides. Structural problems are solved with state of the art x-ray diffraction, or pulsed neutron diffraction facilities, the latter in collaboration with scientists at Argonne's Pulsed Neutron Source (IPNS). In-depth investigations of magnetic properties of well characterized materials are done with a modified Faraday magnetometer coupled to an IBM PC, with extensive data interpretation handled on IBM or Vax mainframes. Although this is a basic research effort, applications in such diverse areas as waste management of radioactive elements or technological uses of high-T_c superconductors are spin-offs of this research.

199 PHOTOCHEMISTRY AND PHOTOPHYSICS OF HEAVY ELEMENTS

Chem.

Phy.

Photo-chem.

The chemical and physical consequences of creating excited electronic states unique to f elements are being investigated in gas, liquid and solid phases. This research effort is defining the forefront of fundamental photophysics and photochemistry studies of transuranic compounds and exploits lanthanide analogs in comparing the behavior of 4f and 5f electron systems. We seek a predictive understanding of the excited-state behavior of these systems using high-resolution laser excitation on nanosecond and picosecond time-scales. Time- and wavelength-resolved fluorescence excitation and emission studies from the ultraviolet to the mid-infrared are carried out by using computer-controlled digital data acquisition and signal averaging systems. Investigations of nonfluorescent systems are carried out by means of thermal lensing and photoacoustic spectroscopies. These studies impact the scientific basis of nuclear waste management and efforts to employ photochemistry to efficiently separate actinide elements and isotopes.

200 SPECTROSCOPY OF THE HEAVIER ELEMENTS

Chem.

Phy.

The lanthanides and actinides are unique in the extent to which important aspects of their electronic structure can be deduced from measurements of the absorption and fluorescence spectra of their compounds. Electronic transitions in each different valence state yield sharp band structure. The energy and intensity of this structure can be interpreted in terms of detailed theoretical models. Opportunity is provided to become acquainted with the theoretical models used to interpret the spectra, as well as the experimental studies which include investigations of crystal spectra at liquid helium temperature and high-resolution spectroscopy in the visible, near-ultraviolet and near-infrared regions. In many areas, the samples of interest are air sensitive and must be prepared and handled by using high-vacuum techniques. Major equipment includes: 1- to 3-meter spectrographs, YAG and N_2-driven tunable dye lasers, as well as standard recording spectrophotometers.

COMPUTING AND TELECOMMUNICATIONS DIVISION (CTD)

The Computing and Telecommunications Division provides a state-of-the-art computing and telecommunications foundation for Argonne National Laboratory's scientific and technical programs and administrative activities. Within CTD, opportunities exist for interns to work in:

- *Computational science and engineering*
- *Distributed computing*
- *Distributed and hierarchical database design*
- *High-performance computing*
- *High-speed networking*
- *Parallel processing*
- *Scientific visualization*
- *Systems programming*
- *Technical Communication*

Four organizational CTD areas share the responsibilities of maintaining this foundation most efficiently: (1) Scientific Applications and Research, (2) Management Information Systems, (3) Computing and Telecommunications Operations, and (4) Planning, Finance, and Administration.

201 SCIENTIFIC APPLICATIONS AND RESEARCH

Comp. Sci.

Scientific Applications and Research develops and promotes research and development opportunities to enhance the Laboratory's expertise and recognition in state-of-the-art computing and telecommunications by:

High Perf. Comp.

Par. Proc.

- Initiating collaborative software development programs with other scientific divisions for adaptation of Laboratory production and state-of-the-art research codes to fully exploit advanced computer architectures. These architectures include current generation supercomputers featuring vector processing and promising parallel-processing concepts.

Sci. Vis.

- Developing strategies for pursuing applications-oriented research within CTD and other scientific divisions that are involved with computational algorithm development, scientific visualization, code parallelizing and vectorizing techniques, and networking for advanced architectures.

- Pursuing actions (both independently and in collaborative initiatives with other scientific institutions) that increase the use of existing ANL computing resources and lead to computational research programs and facility acquisitions that promote further development of ANL as a national center for high performance computing.

- Developing visual techniques, including three-dimensional modeling and animation, for analyzing computational results and data acquired from measurement and sensing equipment.

- Developing advanced data communications techniques and capabilities for use in local area as well as wide area networks for local and distributed scientific and engineering computing applications.

- Developing programs which result in the transfer of advanced computing and telecommunications hardware and software technology to the university and private sectors.

202 MANAGEMENT INFORMATION SYSTEMS

Data base Design

Dist. Comp.

LAN

Management Information Systems (MIS) serves the Laboratory's administrative computing needs by providing administrative and scientific divisions with project managment, business analysis, feasibility studies, commercial software evaluation, systems analysis and design, database design and management, and programming services. MIS also annually produces *A Plan for Administrative Computing at ANL*, which describes all planned and currently operating ANL administrative information systems for the next three fiscal years in the light of current funding recommendations.

In the process of managing these Laboratory administrative computing needs, three MIS sections supervise specific administrative applications. The *Financial Systems Section* oversees and maintains the Laboratory-wide Integrated Financial System as an accounting and planning resource. The *Human Resource Systems Section* is responsible for the personnel payroll and employee health and safety systems. The *Materials and Plant Systems Section* oversees and maintains the procurement, inventory, property, and maintenance control systems. A fourth section, the *Information and Production Services Section* (1) schedules, submits, verifies, and manages the output of administrative batch computing on both IBM and Hewlett-Packard computers and (2) assists users of administrative information with questions about the location or meaning of data within the Laboratory-wide systems.

203 PLANNING, FINANCE, AND ADMINISTRATION

Dist. Comp.

Planning, Finance, and Administration works with all segments of the Laboratory (and especially the Computing Policy Committee) in developing plans, policies, and priorities for research, development, implementation, and protection of computing and telecommunications technologies. Related responsibilities include assembling and publishing the *Guide to Computer Protection* and the annual *Information Technology Resources Longe-Range Plan* and *Site Strategy for Computing Workstations*, working to ensure Laboratory compliance with DOE orders and guidelines (especially Order 1360.1A and 1360.2A, which stipulate software management, implementation, and acquisition for DOE institutions), and management the site-wide unclassified computer protection program and other Laboratory wide activities.

204 COMPUTING AND TELECOMMUNICATIONS OPERATIONS

Comp. Sci.
Dist. Comp.
Data base Design
High Per. Comp.
High Sp. Comp.
High Sp. Net.
LAN
Par. Proc.
Sci. Vis.
Sys. Vis.
Sys. Prog.
Tech. Comm.

Computing and Telecommunications Operations is responsible for providing central computing and telecommunication services to the Laboratory. The four major sections of CTD Operations are Computer Operations, Computer Networking, User Services and Systems Programming.

The *Computer Operations Section* schedules, operates, and maintains Argonne's central computers 24 hours a day, 7 days a week and monitors the operation of many of the Laboratory's networks and external network connections. Services include running computer jobs, setting up input and output devices, performing routine maintenance, monitoring network availability, and adjusting or temporarily reconfiguring the computer system to keep it operating smoothly and continously. This section also operates all the specialized printers and graphical output devices, maintains online and offline data storage and tape libraries, distributes computer documentation, and offers operational services for small computers elsewhere at Argonne.

The *Computer Networking Section* is responsible for the Laboratory's voice and data communications systems, manages the Laboratory-wide network, provides connections to external networks, and provides leadership to users of Laboratory local area networks. Within this section, the Telephone Services Group operates the Laboratory's PBX-based telecommunications system (which provides both voice and data services) and manages the radio, public address, and emergency communications services.

The *User Services Section* provides documentation, courses, and consulting advice on the Laboratory's computer systems and networks for users of the systems. User Services develops and maintains information about available systems, languages, software packages, and library routines; distributes such information through online information and electronic publishing; provides consultants who help users obtain, design, debug, and optimize programs for their specific needs; and offers courses on available interactive systems, high--performance computers, parallel computers, applications packages, and various other aspects of computer usage (such as batch processing, data management, program development, and debugging) that enable Argonne scientists and engineers to take advantage of the full capabilities of the systems.

The *Systems Programming Section* installs and maintains the system software used in the central computers and the software for integrating applications on decentralized divisional computers. Operating system programs and applications programs are evaluated, inspected, modified, and tested to ensure that the general programs supplied by the computer manufacturers meet the Laboratory's needs. The section measures central computing capacity and demand so that it can optimize the availability of resources. It also develops and maintains software that enables both interactive and batch users to benefit from a wide variety of graphics hardware. The Systems Programming Section performs continual assessments and implementation of advanced computing technologies, including vector and parallel processor systems, advanced operating systems for scientific and administrative applications, and data storage devices.

ELECTRONICS DEPARTMENT (EL)

The Electronics Department provides state-of-the-art design, development, and fabrication of custom electronic equipment to support programmatic needs. Electronics Department Personnel are active in proposal preparation and early project planning. They define instrumentation specifications and identify areas where special research and development may be required. They participate in project management, prepare detailed designs, fabricate circuits and instruments, develop software, test the resulting systems, and prepare required documentation.

The Department's activities reflect the main avenues of Laboratory research and development. Typical specialities are electronics for physics and chemistry experiments, instrumentation for accelerators, reactors, environmental monitoring equipment, and biomedical instruments. Particular expertise is available in microcomputers and microelectronics applications, precision measurements, feedback control, computer systems and software, radiation-pulse spectrometry, and many other techniques useful in support of basic and applied research.

205 DATA-ACQUISITION AND CONTROLS SECTION

Elec.
Engr.

Designs and implements computer- and microcomputer-based real-time systems, real-time applications software, distributed-intelligence networks and data links. In addition, designs instrumentation for nuclear reactors, particle accelerators, telemetry systems, and research programs. Calibration services traceable to the National Bureau of Standards are also provided.

206 SYSTEMS ENGINEERING AND SERVICE SECTION

Elec.
Engr.

Applies microcomputers and minicomputers to provide on-line processing capability for scientific and engineering programs. Special purpose interfaces and instruments are designed to fit user needs. This section provides general instrumentation, custom printed circuit boards, operator consoles, and other electronic systems to meet specific experimental requirements. Computer and instrument repair services are also provided.

207 RADIATION DETECTOR INSTRUMENTATION SECTION

Elec.
Engr.
Phy.

Develops new instruments and techniques for radiation detection and imaging, pulse spectrometry, and nondestructive analysis. Systems are developed for applications in synchrotron-light research, neutron scattering studies, environmental monitoring, radiation measurements in vivo, experimental and nuclear physics.

ENERGY SYSTEMS DIVISION (ES)

The Energy Systems Division (ES) at Argonne is a leader in the development of advanced energy and environmental technologies. It is a hands-on, applied research organization with considerable experience in all aspects of technology development, from concept generation to full-scale testing and evaluation. Many projects have near-term commercial potential and are carried out in partnership with private companies. A measure of ES success is the number of our technical innovations that have been adopted by industry.

Our staff is an integrated, experienced team of 90 professionals who bring together expertise from many engineering and scientific fields. Included are chemical and mechanical engineers, chemists, physicists, earth scientists, economists, and transportation analysts. The ES staff is organized into two groups. One focuses on applied research on geoscience problems related to resource use and on engineering development of biochemical, thermal, mechanical, and chemical processes; the other performs technical and economic evaluations of energy and environmental technologies.

THE MINORITY ENERGY RESEARCH PROGRAM

The Minority Energy Research Program, managed by Argonne National Laboratory for the Office of Minority Economic Impact of the United States Department of Energy, is concerned with conducting research that will help the Secretary of the Department to design and implement programs that will assist minority energy consumers and minority owners of energy businesses. The key objectives of the Program are (1) to assemble and analyze a comprehensive database concerning minority energy consumption and expenditures; (2) to advise the Secretary on the impact of energy policy and programs on minority energy use and expenditures; and (3) to conduct research that will aid minority-owned energy business.

208 MINORITY IMPACT - DATA ANALYSIS

Comp. Sci.
Econ.

For assembling, analyzing, and integrating a diverse set of transportation and residential energy databases that can subsequently be used in impact assessments. Present emphasis is on statistical analysis and on identifying statistical tools that will facilitate more integrated use of diverse databases.

Soc. *Stat.*

209 MINORITY IMPACT - IMPACT ASSESSMENT

Pol. Sci.

For identifying energy issues of greatest relevance to minority groups and for assessing the impact of energy policy and programs on those groups.

Soc. *Geog.* *Urban Planners* *Econ.*

210 MINORITY IMPACT - BUSINESS ASSISTANCE

Finan.
Mktg.

For identifying issues of greatest concern to minority owners of small energy-related businesses, and for conceptualizing connections between them and minority energy consumers.

Urban Planners

RECLAMATION ENGINEERING AND GEOSCIENCES

The Reclamation Engineering and Geosciences Group performs analytical and experimental studies concerned with the management of energy and mineral resources and with the development and deployment of related technologies. Major activities of the group include: acquisition of field and laboratory data for solution of problems of geoscience and engineering; analysis of geoscience data to support the design and deployment of energy technologies; and the development and evaluation of mathematical models of geophysical and geotechnical systems.

211 GEOLOGIC AND HYDROLOGIC ENGINEERING

Civil Engr.
Geol.
Hydrol.

Studies of the interaction between energy-extraction operations and energy-production systems and the environment often involve investigations related to geologic or hydrologic engineering. Current studies deal with development of statistical methods for measuring the effectiveness of site-characterization methods, groundwater modeling, and field measurements associated with environmental compliance at energy R&D facilities.

Geohydrol. *Chem. Engr.*

212 GEOLOGICAL/GEOPHYSICAL RESEARCH

Geol. Engr.
Geophy.

Studies of energy resources involve geological and geophysical data acquisition, analyses, and interpretation, frequently through some form of modeling. Current studies deal with: continental rift resources, lithospheric flexure, basin hydrodynamics, earthquake prediction, deep seismic reflection sounding of continental rifts, seismic reflection/refraction processing techniques, and field investigations of environmental or hydrological issues.

Geosci. *Hydrol.* *Geostatics*

213 ENVIRONMENTAL RESEARCH AIMED AT SOLVING PROBLEMS RELATED TO ENERGY DEVELOPMENT

Bio.
Bot.
Envr. Sci.

The overall objective of the program is to plan and conduct field and laboratory research efforts to develop and test new and improved land reclamation methods. The program will provide quantitative environmental data and scientific evidence on the impacts of energy production and transportation on the environment. The program consists of the following research areas: (1) Vegetation and Soils, (2) Stream Crossing, (3) Wetlands, (4) Erosion Control, (5) Land Rehabilitation, (6) Hydrology and (7) Sediments.

Ecology *Hydrol.* *Soil Sci.* *Civil Engr.* *Geotech. Engr.*

CENTER FOR TRANSPORTATION RESEARCH

The Center for Transportation Research (CTR) conducts applied research on advanced transportation technologies and their energy, economic, and environmental impacts for the U.S. Department of Energy. A broad spectrum of technologies are being researched; some examples include alternative-fueled vehicles, magnetically levitated high speed vehicles, oxygen-enriched engines, and environmental impacts of the transportation of hazardous materials. Ongoing work also includes projects of energy use and transportation demand under different future scenarios, environmental assessments and modeling of existing and new technologies, and issues and strategies for a transition to alternative fuels. Due to the breadth of current research topics, CTR is interested in attracting both students and faculty from a diverse set of disciplines to contribute to our research efforts.

214 ALTERNATIVE FUELS FOR TRANSPORTATION

CTR is conducting technical, economic, policy, and environmental analyses for a transition to non-petroleum fuels for the transportation system. Projects span light and heavy duty vehicles and buses, and include fleet demonstrations. Analysis of alternative transportation fuels in CTR includes: (1) assessment of engine, vehicle and fuel supply technologies, (2) assessment of the properties of fuels, their combustion products and atmospheric side effects, (3) econometric analysis of consumer response to the cost changes of fuels and vehicles when adopting alternative fuels, and (4) economic assessment of policies designed to promote the introduction of alternative fuels. Relevant disciplines include: mechanical and chemical engineering, economics, marketing, environmental sciences/engineering, chemistry, biology, political sciences, statistics, computer science. Two specified examples of ongoing projects are listed below.

215 ALTERNATIVE TRANSPORTATION FUELS - VEHICLE AND FUELS CHARACTERIZATION

Chem. Engr.

Mech. Engr.

Studies the attributes of engines and fuel systems for various fuels and technologies and develops comparisons of advantages and disadvantages of each. Emissions, energy consumption, power density and other measures are used as a basis of comparison. May also study fuel processing and transportation systems such as refineries, pipelines, and ships. May estimate costs of technologies, working with economists.

216 ALTERNATIVE TRANSPORTATION FUELS - ECONOMIC ASSESSMENTS

Econ.

Studies consumer responses to vehicle and fuel characteristics, including price changes and factors such as performance and safety. Study policy questions including issues of short run costs vs. long-run savings induced by inter-fuel competition. Works with engineers to develop costs estimates for new technologies.

217 THE MAGLEV PROGRAM

Phy.

Elec. Engr.

The Center for Transportation Research is currently conducting a study of magnetically-levitated vehicle technology and what role that technology could serve in the U.S. transportation system. Both normal and superconducting technologies are being considered and evaluated. A plan for a major U.S. research and development program leading to a commercially viable system design is being formulated. A broad range of talents are required to perform the analyses currently in progress and those anticipated as the program continues to develop. These include dynamics, civil, mechanical and electrical engineering, physics, systems analysis, economics, and city and transportation planning.

218 OXYGEN ENRICHED DIESEL ENGINE RESEARCH

Mech. Engr.

The purpose of this project is to investigate the technical and economic feasibility of using oxygen-enriched air to increase the thermal efficiency and to decrease emissions from a diesel engine.

219 EXPERIMENTAL DATA COLLECTION

Mech. Engr.

Mechanical Engineering Assistant for acquiring engine test data using high-speed data acquisition system and analyze the data. Graduate or senior or level undergraduate Mechanical Engineer.

220 ANALYTICAL ENGINEER

Mech. Engr.

Mechanical Engineering or computer systems engineer to conduct simulation studies of engines and vehicle systems.

PROCESS EVALUATION GROUP

221 SPECIAL PROJECTS AND INDUSTRIAL APPLICATIONS GROUP

Chem. Engr.
Comp. Sci.
Econ.
Math.
Mech. Engr.

Several technology assessment and energy policy studies are underway. Specific projects include: technical and economic analysis of biomass technologies, covering conventional and advanced biomass production and conversion technologies; evaluation of a new coal-oxygen process for CO_2 production for enhanced oil recovery; assessment of energy storage technologies in transportation applications; evaluation of electric utility load management options, including a survey of cool storage applications for the Electric Power Research Institute (EPRI); and several financial analysis studies, including the financial analysis of the Great Plains Coal Gasification Project for DOE and a financial simulation of the Prototype Breeder Reactor for EPRI.

PROCESS AND SYSTEMS ENGINEERING

222 DEVELOPMENT OF ADVANCED ENVIRONMENTAL CONTROL TECHNOLOGY

Chem. Engr.
Chem.
Envr. Sci./Engr.
Mech. Engr.

The objective of this project is to develop advanced techniques for the control of air emissions from the combustion of fossil fuels. Many of the technologies are also applicable to systems that involve combustion of municipal waste or hazardous chemical wastes. Currently, the program focus is on technologies that integrate control of NO_x, SO_2, and particulate matter into one system replacing the current, more expensive approach of separate operations in series. Activities include laboratory research in aqueous scrubber chemistries, dry sorbent/additive techniques, and spray drying. State-of-the-art laboratory facilities, experimental design and analytical techniques, and computerized data collection/analysis procedures are employed.

223 RECOVERY OF HYDROGEN AND SULFUR FROM H_2S USING A MICROWAVE-INDUCED PLASMA

Chem.
Chem. Engr.
Elec. Engr.
Envr. Sci./Engr.

The objective of this project is to develop a new waste treatment technology that recovers hydrogen plus sulfur from industrial hydrogen sulfide waste streams. Laboratory experiments are being conducted to investigate the effects of a "cold" microwave-induced plasma on both pure H_2S and mixtures of H_2S with other gases expected in an industrial (e.g., refinery) waste stream. Parallel engineering evaluations are conducted to identify potential commercial applications, develop process configurations, and estimate process economics.

WASTE AND SAFETY ENGINEERING

224 SAFETY ENGINEERING

Chem. Engr.
Civil Engr.
Envr. Engr. *Mech. Engr.*

Industrial processes are being analyzed to develop optimal design and operation from a safety system engineering perspective. The safe handling, transportation and utilization of hazardous materials are being studied. The safety system approach is also being used to optimize the treatment, storage, and disposal of hazardous waste.

225 WASTE MANAGEMENT

Chem. Engr.
Civil Engr.
Envr. Engr.
Mech. Engr.

Research and development for the treatment of waste includes chemical, physical, biological and thermal processes. Laboratory studies are underway in these areas to discover and develop innovative technologies for waste treatment. Types of waste being considered include hazardous waste, mixed waste, and wastes that are generated by municipalities. The minimization of the generation of these wastes is also being analyzed to develop methods, processes and related technologies to reduce or eliminate their environmental liability.

EXPERIMENTAL SYSTEMS ENGINEERING

226 THERMAL SCIENCES

The overall objective of this program is to conduct applied research in heat and mass transfer. The program focuses on the study of underlying mechanisms in heat and mass transfer enhancements, fouling, and heat and mass transfer in multiphase flow. The research outcome consists of validated models and design methods for high performance thermal systems. Experimental and analytical work is conducted at Argonne and at supporting subcontractors facilities. Currently this task encompasses parts of two Department of Energy programs: Heat and Mass Transfer Technology, sponsored by Conservation and Ocean Thermal Energy Conversion, supported by Renewables.

227 SYSTEMS, ANALYSIS AND MODELING

Chem. Engr.
Mech. Engr.

Several computer projects exist primarily in the area of combustion, radiation heat transfer, and multiphase flow. Usual work involves either the development of new computer programs or analysis problems using existing computer codes. Level of training should be at least a B.S. degree.

228 MAGNETOHYDRODYNAMICS/MHD PROPULSION

A research and development program has been structured to address critical technical issues that affect MHD propulsor performance. The primary goal of the proposed program is to investigate the steady-state and transient performance of MHD thrusters over broad parametric ranges and to develop validated scaling relationships and models for projecting performance to geometical and operational parametric ranges of interest for full-scale systems. The 3-D modeling activities being pursued are critical to isolating and quantifying the magnetohydrodynamic phenomena and loss mechanisms. A secondary goal is to develop preliminary data on the acoustic noise levels attributable to an MHD thruster and in so doing, ascertain the degree to which MHD thrust is inherently quiet. A large sea water test facility is being built which will be coupled to the ANL 6-T magnet (world's largest dipole saddle) to provide a test facility for investigating the magnetohydrodynamic-performance of prototype thruster channels.

Chem. Engr.
Elec. Engr.
Mech. Engr.
Magneto/fluids mech. model.

229 NATIONAL ENERGY SOFTWARE CENTER

The National Energy Software Center serves as the software management and information center for the U.S. Department of Energy and Nuclear Regulatory Commission. The Center collects, reviews, tests, packages, and distributes software developed under DOE and NRC sponsorship. The Center's library currently contains over 1500 programs. About 150 programs are added to the collection each year. The Center also coordinates the exchange of NESC software with other governmental organizations and the OECD Nuclear Energy Agency Data Bank. Other NESC activities include development of guidelines for sharing software and standards for software review, packaging, and distribution.

Comp. Sci.
Engr.
Info. Sci.
Math.
Nucl. Sci. *Phy.*

ENGINEERING PHYSICS DIVISION (EP)

The multi-faceted division is involved in a wide array of space, defense, RF superconductivity, nuclear fission and fusion energy production, and advanced energy systems research and development activities. Principal current program topics include nuclear and non-nuclear space electric power plants, neutral particle beams for strategic defense applications, fusion engineering and physics, aerosol sciences, nuclear reactor physics and its applications, liquid metal reactor systems and components, and low-enrichment uranium fuel.

Problems in fission reactor physics are studied by use of critical reactor assemblies, application of reactor physics theory and codes, measurement of the microscopic nuclear parameters needed in the analyses, and development of the instrumentation for experiments. For the fusion reactor, studies of plasma physics and fusion reactor neutronics are in progress.

A flexible fast-critical facility, known as the Zero Power Physics Reactor (ZPPR), provides for direct observation of the characteristics of fast reactors. The Division utilizes an 8-MeV particle accelerator to generate neutrons and thus provide basic nuclear information on the physical foundations of the chain-reacting system.

Other Division programs are directed toward the study of reactor safety research in which the main emphasis is in engineering and physical model developments for hypothetical accidents for advanced reactors. For the next generation of fission reactors, the advanced system neutronics of the core, blanket, and fuel-cycle are developed.

230 SPACE POWER

Elec. Engr.
Mech. Engr.
Nucl. Engr.

This project involves the development of designs of power systems capable of producing multimegawatt levels of electric power in space. Need for such large amounts of steady-state and burst power is foreseen for a number of defense and civilian missions in the next decade and beyond. For large power systems, nuclear power has been shown to be an optimal choice, often in conjunction with chemical power systems. Designs are developed for all of the power system components including the nuclear reactor, the power conversion devices, energy storage devices, heat rejection devices and power conditioning. The microgravity environment of space imposes stringent design requirements on the system as does the necessity of disposing of very large amounts of excess thermal energy by radiation. The design effort is supported by research and development activities on several of the key technology areas including neutronics and control, energy storage, and nuclear fuel development.

231 APPLIED ACCELERATOR TECHNOLOGY

Comp. Sci.
Elec. Engr.
Phy.

These activities entail the development of advanced accelerator technology and require computer programming support in the following general areas:

(1) design and development of user friendly interfaces for accelerator data acquisition systems,
(2) design and development of control systems for advanced accelerators, and
(3) programming of mathematically complex codes which model the dynamics of charged particle beams.

232 FUSION ENGINEERING RESEARCH

Chem. Engr.
Elec. Engr.
Mech. Engr.
Nucl. Engr.

This project involves planning and carrying out an experimental program to study the interactions of large magnetic fields with liquid-metal coolants proposed in fusion reactor blanket designs. The experimental project primarily involves design of test sections, development of velocity instrumentation, development of computer software to gather, store and reduce experimental data, and the analysis of experimental results. Analytical activities consist of developing predictions for the velocity, pressure and voltage distributions in the flowing metal and are being carried out in direct support of the experimental program.

233 AEROSOL SCIENCES

Chem. Engr.
Elec. Engr.
Envr. Engr.
Mech. Engr.
Phy.

Participants' primary responsibility will be to contribute to experimental investigations and theoretical modeling in the fields of basic and applied aerosol science. Opportunities also exist in the areas of computerized data acquisition and data reduction. Research applications include aerosol generation, transport, pollution control, sampling and analysis for both nuclear and fossil power systems. Additional research areas involve the development of novel devices to disperse or collect particles or to develop instrumentation to measure aerosol parameters, pulsed corona applications, and spray generation and characterization. Basic areas of research include electrostatic particle charging, particle formation, transport, agglomeration, deposition and adhesion mechanisms; radiative heat transfer in particle laden gases; particle filtration; material erosion by aerosol impaction; and aerosol-vapor interactions.

234 COMPUTER SCIENCE IN SUPPORT OF FUSION ENGINEERING RESEARCH

Comp. Sci.
Elec. Engr.

You will be part of a diversely educated team of researchers composed of students, technicians, a university professor, and Argonne staff members. You will contribute to the team in a number of areas, but primarily, will be responsible for a system of data reduction and plotting software. This software system is the workhorse tool used by the team to evaluate, and interpret the results of the experimental program, called ALEX (Argonne Liquid-Metal Experiment). Specifically, task assignments will include software revisions to develop and apply digital signal processing techniques to help understand Liquid Metal MHD phenomena which have been observed in the ALEX experiment. Techniques which are being used include fast Fourier transforms, signal auto-correlation, digital filtering, and pattern recognition. You will also be responsible for a number of enhancements to the system to improve the methods of data evaluation, and for modifying and upgrading the system for future experiments.

235 COMPUTER AIDED ENGINEERING

Elec. Engr.
Mech. Engr.
Nucl. Engr.

This area encompasses engineering done with the aid of special computer linked devices, computer-aided design (CAD) and computer-aided manufacturing (CAM). The Computer Aided Engineering Center (CAE) equipment uses Intergraph and AutoCad systems.

236 ADVANCED COMPUTING

Comp. Sci.
Mech. Engr.
Nucl. Engr.
Phy.

This research involves applying new advances in computing, such as parallel processing, rule-based information systems, graphics in a distributed processing environment, and alternate programming models (e.g., object-oriented programming), to the development and application of improved system analysis and simulation capabilities. Research activities have been performed for both DoD (parallel simulations for SDI) and DOE (energy systems research and development). Activities for participants include algorithm parallelization, developing computer models for advanced energy system components, and programming general-purpose graphics libraries for over-a-network visualizations. Familiarity with C, FORTRAN, and UNIX are desirable.

237 MONTE CARLO ANALYSIS METHODS DEVELOPMENT

Comp. Sci.
Math.
Nucl. Engr.
Phy.

The Monte Carlo methods provide an exact but expensive technique for the computer solution of the Boltzmann equation (which governs average neutron behavior in a nuclear reactor). A Monte Carlo method is being used to test the accuracy of a number of less expensive, but approximate solution techniques for the Boltzmann equation. The research project will involve performing one or more sets of comparison calculations between Monte Carlo and approximate techniques and drawing conclusions from the results. The participant will have an opportunity to learn and apply reactor physics, mathematics, and Monte Carlo theory. Some knowledge of FORTRAN is required.

238 FUEL CYCLE SYSTEMS

Chem.
Chem. Engr.
Math.
Nucl. Engr.
Phy.

During the operation of a nuclear reactor, certain uranium isotopes are burned and plutonium isotopes are produced. The changes in isotopic composition with burnup of the fuel is a measure of the radiation history in the reactor. Computation and experiments indicate that there exist relationships between isotopic concentrations which have a predictable, functional behavior over a broad range of reactor operating conditions and burnup. The purpose of this study is to determine these plutonium and uranium isotopic correlations and measurement techniques as a material control process and as a safeguard material accountability measure in the dissolver stage of the nuclear fuel cycle. The study includes the design of a mini-computer system as a field instrument for implementation at the reprocessing operations.

239 ZERO POWER PHYSICS REACTOR (IDAHO)

Comp. Sci.

Engr. Phy.

This is the world's largest fast reactor critical facility and it is operated by the Engineering Physics Division in Idaho. See ARGONNE-WEST for a description of the research at the reactor.

Mech. Engr. *Nucl. Engr.* *Phy.*

240 PLASMA PHYSICS

Comp. Sci.

Nucl. Engr.

Phy.

Engineering analyses of plasma behavior in fusion reactors are performed using computer simulation. Studies include fusion burn dynamics, MHD equilibria, impurity control, plasma-wall interactions, neoclassical transport and reactor startup and shutdown studies. Background in plasma physics and experience with computer programming are desirable.

241 FISSION REACTOR ANALYSIS COMPUTER CODE DEVELOPMENT

Comp. Sci.

Nucl. Engr.

A group in the Engineering Physics Division develops and maintains a number of large, exportable computer programs which are buased on neutron diffusion and transport theory. These codes employ a variety of approximate methods, usually based on discrete forms of differential equations, to perform static and time-dependent calculations and are fundamental production tools of fission reactor analysis. Possible areas for projects are: performing benchmark calculations, programming additional features, and implementing codes on new machines. Participants should have a knowledge of FORTRAN; some understanding of reactor physics is helpful but not a prerequisite.

242 FAST-NEUTRON PHYSICS AND NUCLEAR DATA DEVELOPMENT

Comp. Sci.

Math.

Nucl. Engr.

Phy.

A comprehensive program of fast-neutron physics for basic and applied science is carried out at the Fast-Neutron Generator (FNG). The work involves experiments, data analysis and physical interpretations associated with the study of a wide range of nuclear reactions induced by neutrons at energies from a few keV up to 20 MeV. This energy range is of great importance for many applications (fast-fission reactors, nuclear fusion, radiography, nuclear waste disposal, radiation protection, etc.). The long-term objective of this research program is to provide detailed quantitative information for all open reaction channels across the entire periodic table, and to establish a complete evaluated database which can be used with confidence in engineering applications, in confirming nuclear theories and in developing effective nuclear models for use in computer studies of nuclear systems. An important part of this effort is the development of new methods for measuring and analyzing nuclear data. Experiments are done on the FNG tandem accelerator and they employ a variety of equipment and methodologies for detecting neutrons, beta particles, alpha particles and gamma rays. Data analysis involves the conversion of measured radiation spectra to such fundamental constants as reaction cross sections, radiation decay branching parameters, etc. Nuclear models are used to interpret these results. Data measured in this laboratory, and elsewhere in the world, are evaluated using sophisticated statistical techniques in order to provide recommended values which are documented in national and international evaluated nuclear data files. This work requires a general knowledge of physics laboratory practice, some background knowledge of nuclear physics and nuclear measurement techniques, good analytical skills, and experience with personal computers and computer work stations. A knowledge of FORTRAN is also desirable. Work on independent projects with a modest level of supervision is encouraged. All work is published in journals, laboratory reports and conference proceedings.

243 MAGNETOHYDRODYNAMIC SEAWATER PROPULSION

Elec. Engr.
Mech. Engr.
Nucl. Engr.

This project involves planning and carrying out an experimental program to study the interactions of large magnetic fields with sea water in ship propulsion thrusters. Such thrusters would provide a significant breakthrough in marine propulsion. The experimental project primarily involves utilization of a large superconducting magnet, cryogenic system, power supply, and instrumentation to collect data for various parameters of interest. These data will then be used to quantify and extrapolate performance for prototypical thrusters.

244 COMPUTER SCIENCE IN SUPPORT OF MHD SEAWATER PROPULSION

Comp. Sci.
Elec. Engr.

The participant will be responsible for a system of data acquisition, real time monitoring, data reduction, and analysis. This hardware/software system is the tool used to gather, evaluate, and interpret results from the magnetohydrodynamic seawater propulsion experiment. Specifically, the participant will be responsible for a number of enhancements to the system to improve methods of data evaluation and real time monitoring.

ENVIRONMENT, SAFETY AND HEALTH DEPARTMENT (ESH)

The Environment, Safety and Health Department is responsible for: (1) providing technical support to assure a safe work environment for Argonne employees, (2) providing environmental surveillance and effluent monitoring to assure adequate environmental protection and (3) for conducting a wide variety of research and development activities related to the practices of health physics, industrial safety, industrial hygiene, environmental protection, decontamination and decommissioning and other health and safety activities. Personnel of the Department are engaged in the wide scope of activities required to make recommendations for and maintain safe work practices and conditions throughout the Laboratory. Activities include safety engineering, health physics services, industrial hygiene services, personal monitoring, internal dosimetry, environmental protection, industrial hygiene and safety analyses.

245 INDUSTRIAL HYGIENE

Bio.
Chem.
Envr. Sci.
Phy.

A wide variety of potential occupational health hazards are evaluated at research and support activities. Exposures to solvents, gases, vapors, dusts, and mists are measured using a variety of direct-reading instruments and personal sampling devices. Laboratory analyses are performed on workplace, environmental, and biological samples. Other activities involve exposure surveys for noise, ultra-violet light and microwaves, selection, fit testing and user training of respiratory protective devices, and particle collection efficiency measurements of high performance air cleaning systems. Projects are available concentrating on a specific aspect of occupational health. A wide variety of instrumentation is used, including infrared, electrochemical cell and photoionization type gas and vapor monitors, aerosol photometers, data loggers, noise and microwave meters, and laser-based fibrous aerosol monitors. Optical and electron microscopy is used for particle and fiber analyses.

246 INTERNAL DOSIMETRY

Chem.
Comp. Sci.
Phy.

This group is responsible for determining whether an ANL employee received any internal radioactive contamination; and, if so, the extent of the potential exposure from that contamination is determined. Available research projects are of three types: analytical radiochemistry, instrumental techniques for measuring low-level radioactivity (including body radioactivity counting), and computer programming and analysis of empirical data. Major equipment includes: whole-body counting facility; liquid-scintillation spectrometers; alpha and gamma spectrometer systems; multichannel analyzers, MicroVax II supermicrocomputer, microcomputers, and computer terminals.

247 ENVIRONMENTAL PROTECTION

Bio.
Chem.
Comp. Sci.
Envr. Sci.

The section is responsible for the monitoring of radioactivity around the Laboratory. This is accomplished by the application of radioanalytical separation techniques to environmental materials such as air, water, soil, plant, benthos, foodstuffs, etc. Related to this is the use of instrumentation for the measurement of very low levels of radioactive materials. Available research projects include low-level radiochemical analysis, computerized data management, thermoluminescent dosimetry (TLD) studies at environmental levels and pathway analysis of the movement of radionuclides through the environment.

248 HEALTH PHYSICS

Chem.
Envr. Sci.
Nucl. Engr.
Phy.
Radio. Phy.

This group is involved in all phases of the radiation monitoring, hazard evaluation, dosimetry, exposure control and experiment review activities connected with ANL programs which use radiation sources. In addition, it provides radiological characterization and assessment studies and decontamination and decommissioning efforts for formerly utilized nuclear facilities. Specific areas of research and/or development activity which are presently of interest, include the following: radiation dosimetry studies; continuing stray neutron energy spectrometer studies around ANL accelerator facilities; analysis of various Bonner sphere unfolding codes for neutron energy spectra; development of monitoring techniques for transuranic elements; determination of the sensitivity of stack effluent monitoring equipment for detection and measurement of reactor and hot cell effluents; development of Health Physics training courses; qualitative and quantitative studies of the activation of accelerator components and surroundings by intense particle fluxes; development of techniques for radon and radon daughter monitoring; determinations of field techniques for radiological characterization of soils and other contaminated materials; acquisition of improved field spectrometry techniques; development of improved radiation survey instrument calibration techniques; development of state-of-the-art microprocessor-based survey instruments; implementation of an ALARA program; and evaluations of the management of Health Physics records. A wide variety of radiation instrumentation is available including state-of-the-art survey and laboratory instrumentation. The latest in hyperpure germanium spectrometry systems as well as an anticoincident annulus NaI system constitute but a part of the instrumentation inventory. Three equipped mobile laboratories are used for field measurements and emergency response capabilities. A wide variety of research and development experiences are possible.

ENVIRONMENTAL ASSESSMENTS AND INFORMATION SCIENCES DIVISION (EAIS)

The Environmental Assessment and Information Sciences Division has developed a broad program of interdisciplinary, applied research and development, undertaken from a system's perspective. The staff addresses a wide range of issues associated with energy technologies, energy and enviornmental policy, and environmental and societal effects of resource and industrial development. Environmental and resource assessments are conducted by professionals with expertise in the geohydrological, physical, social and ecological sciences and in radiological and health risk assessment. Our policy staff consists of economists, sociologists, land use planners, and archaeologists, and provides sophisticated analyses of government policy and strategy options. Special areas of interest include labor and regulatory economics, cost-benefit analysis, perceived risk analysis, and assessment of cultural resources. We are experienced in building multidisciplinary technical teams for specific environmental projects, since many of our programs require integration of a wide range of skills.

The Advanced Computer Applications Center within EAIS performs a variety of applications-oriented computer research based on emerging hardware and software technologies. The Center focuses on parallel processing machines, advanced scientific and engineering workstations, powerful graphics workstations, and high-speed networking systems. The concept of distributed computing is exploited to enable optimal interconnection and efficient use of these machines as complementary tools for problem solving. The Center is part of the Argonne Advanced Computer Collective.

INFORMATION SCIENCES

249 ECONOMICS AND LAW

The effects of energy and other related problems are investigated at the local, regional and national levels. The economic and legal implications of public policy for energy development are studied, and methods for mitigating undesirable consequences are assessed. The projects usually include benefit/cost, financial, statistical and institutional analyses.

Comp. Sci.
Demogr.
Econ.
Geogr. *Public Admn.* *Sociol.* *Urban Planning*

250 SYSTEMS SCIENCE

Energy technologies (e.g., fossil technology, environmental contral technology) are evaluated and compared as to cost, reliability, environmental effects, and implications for health and safety. Decision-analytic techniques are used in solving decision problems (e.g., R&D portfolio selections, project prioritization, energy technology comparisons).

Comp. Sci.
Envr. Sci.
Ind. Engr. *Mech. Engr.* *Nucl. Engr.* *Operations Research*

251 ADVANCED COMPUTER APPLICATIONS CENTER

The types of problems currently under investigation include large-scale simulation modeling, large-scale data management, contingency analysis, decision analysis, computer throughput improvement, intelligent and graphical man/machine interfaces, development environments, high-resolution graphics, and computer aided software engineering (CASE) tools. Approaches used for obtaining improved solutions for problems in these areas include object-oriented programming, artificial intelligence, expert systems, fine- and coarse-grained parallelism, multiprocessor computer architectures, and distributed systems.

Comp. Engr.
Comp. Sci.
Decision Theory

Infor. Sci.   *Operation Research*

252 ENERGY POLICY

Federal, state, and local policies to protect the environment and to make efficient use of natural resources are evaluated as to their effect on the implementation and use of energy systems. Interdisciplinary approaches are used to analyze the effects of policy changes on energy systems and environmental quality.

Econ.
Envr. Sci.

Ind. Engr.   *Mang. Sci.*   *Public Admn.*

ENVIRONMENTAL ASSESSMENT AND RESOURCE MANAGEMENT

253 ATMOSPHERIC SCIENCES

Construction and operation of energy technology systems and other industrial and regional activities are evaluated to assess impacts on ambient air quality, climate, meteorology and acoustic environment. The effectiveness of control technologies and related government regulations in mitigating these impacts is also evaluated. New and improved methods of modeling environmental transport and transformation processes are developed as part of this work.

Air Qual.
Comp. Model.
Envr. Engr.

254 MATHEMATICAL AND COMPUTER MODELING

Analytical and numerical modeling of current environmental problems are performed. Computer algorithms are developed and databases are collected in support of environmental research and remedial action activity. Independent studies in numerical, analytical, and statistical methodologies are undertaken to facilitate a clear description and understanding of natural and imposed impacts on the environment.

Comp. Sci.
Geol.
Hyd.   *Math.*

255 ENVIRONMENTAL COMPLIANCE ACTIVITIES FOR REMEDIAL ACTIONS AT FORMERLY UTILIZED ATOMIC ENERGY COMMISSION SITES

The Division is responsible for providing oversight review, technical and regulatory consultation and recommendations to DOE for the planning and execution of the entire NEPA (National Environmental Policy Act) process to ensure that environmental matters are taken into consideration in the Department of Energy's efforts to decontaminate many sites used in the 1940's and '50's under the old Manhattan Engineer District (atomic bomb project). These sites require environmental documentation as set forth by both NEPA and the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA). The activities include the preparation of environmental assessments, environmental impact statements, remedial investigation/feasibility studies, engineering evaluation/cost analyses, and baseline risk assessments.

Ecol.
Econ.
Envr. Engr.
Envr. Sci.
Health Phy.

Geol.   *Nucl. Engr.*   *Soci.*

256 HAZARDOUS WASTE ASSESSMENT PROGRAM

Comp. Sci. *Envr. Chem.* *Envr. Engr.* *Geol.*

The Division also conducts planning and execution of CERCLA/SARA as an integral part of a hazardous waste assessment program for the U.S. Army and Navy. The work includes analyzing waste management practices at different sites particularly regarding their effect on contaminant concentrations in soils, surface water and groundwater. The impact of federal, state, and local regulations on waste management is also analyzed. This includes regulations which define hazardous waste and appropriate concentration limits in water and soil. Preliminary assessments, remedial investigations, feasibilty studies and risk assessments are conducted.

Studies to minimize hazardous waste production at different installations are carried out. Factors considered in the studies include changes in production and processing methods, substitution of products and chemicals used in processes, and changes in waste management practices. Cost factors are also included.

257 SOCIAL AND NATURAL RESOURCES

Comp. Sci. *Demogr.* *Econ.* *Forest.* *Geogr.* *Public Admn.* *Soc.* *Urban Planning*

Human interactions with the natural environment are studied using techniques from ecology, human ecology, demography, sociology, archaeology as well as techniques from other natural sciences, economics and planning. Research focuses on disruption to the human and natural environment of such diverse topics as multiple small hydro development effects on fisheries to social and economic consequences of creating radioactive waste facilities. Other research topics being studied include optimization of national park boundaries, inclusion of social and environmental variables in geographic information systems, epidemiology, demographic transition of aging populations, cumulative biological impacts, social aspects of reforestation, public involvement and biodegradation of waste.

258 RADIOLOGICAL ENVIRONMENTAL RISK ASSESSMENT

Health Phy. *Math.* *Nucl. Engr.* *Phy.*

This activity involves the assessment of radiological impacts resulting from the releases of radioactive materials from transportation of radioactive nuclear waste materials. The assessment requires the modeling of the transport of radioactive materials via various environmental pathways that would eventually lead to radiation exposure to humans. Modeling includes computer simulation of radiation transport, atmospheric dispersion, radionuclide pathways, and radiation health effects.

259 ENVIRONMENTAL SYSTEMS PLANNING AND COMPLIANCE

Engr. *Envr. Engr.* *Phy. Sci.*

Both multi-media and medium-specific approaches are taken to assess and solve environmental problems that exist at federal facilities. Specific activities include both analytical studies and field work such as development of handbooks and guidance materials; audits of environmental compliance at federal facilities; presentation of workshops on environmental laws, regulations, and compliance; development of emission inventories; development of database management and expert computer systems for environmental information and permits; and preparation of NEPA documents and management of the NEPA process for specific projects.

260 COMPUTER MODELING OF RADIOLOGICAL ENVIRONMENTAL ASSESSMENT

In an effort to assist DOE in establishing soil guidelines, a microcomputer program has been developed. The program has incorporated DOE criteria for residual radioactive materials in soil. Various environmental pathways have been developed, and currently are being updated, for the code. These updates include the refinement of dose factors and inclusion of radon pathways to the exposure to humans.

Health Phy.
Math.
Comp. Sci.
Nucl Engr. Phy.

261 SYSTEMS ECOLOGY

Analyses are conducted on the effects of human activities on aquatic, terrestrial, and wetland ecosystems. These include analyses of ecological communities, plant and animal populations, threatened and endangered species, and cumulative impacts. Mitigation strategies such as habitat reclamation and restoration are developed to reduce the projected impacts of development. Ecological information is analyzed using statistical techniques, modeling, and geographic information systems.

Ecol.
Envr. Sci.
Bio stat.
Model. GIS

262 INTERNATIONAL COAL AND ENVIRONMENTAL STUDIES OFFICE

The International Studies Office coordinates all energy and environmental planning activities within the EAIS Division, in support of the U.S. Department of Energy (DOE) Office of International Affairs, the Agency for International Development, the World Bank, and other organizations that sponsor specific EAIS Division programs with a significant international dimension.

Study areas:

1. Energy planning, assessment, modeling, and training.
2. Renewable resource utilization and conservation.
3. Hazardous waste planning and assessment.
4. Environment planning, assessment, modeling, and training.
5. Fossil energy research, planning, development, analysis and assessment, technology initiatives, especially Clean Coal Technology applications.

Bus. Admn.
Chem. Engr.
Econ.
Envr. Engr.
Intl. Relat.
Pol. Sci.

ENVIRONMENTAL RESEARCH DIVISION (ER)

Research activities in this division include a broad spectrum of fundamental and applied investigations into the functioning of environmental systems, particularly in response to anthropogenic stresses. Consequently, the information derived from the various research projects addresses critical environmental issues that face society. Current emphasis is on the environmental effects of hazardous wastes (e.g., identification, amelioration, and remediation) and atmospheric responses to energy production and use (e.g., induction of acidic rain, alteration of global climate). The Division is organized by into two scientific sections (Atmospheric Research and Terrestrial Research), each with several research groups, as well as three major additional program groupings (Environmental Management and Surveys, Photophysics and Photochemistry, and Radiation Physics). An interactive and collaborative approach to the investigation of these complex environmental issues is the hallmark of the Division.

ATMOSPHERIC SECTION

Research activities include investigation of the physics and chemistry of the lower atmosphere, particularly with regard to the processes of transport, chemical transformation, diffusion, and deposition of airborne trace substances. Related activities involve studies of climate change and aquatic environments in freshwater lakes. Factors that influence the behavior of pollutants are measured with a view toward the development of descriptive theoretical and numerical models. Particular attention is paid to the changes in the atmosphere that are brought about by human activities, such as emissions from the burning of fossil fuels.

263 ATMOSPHERIC PHYSICS AND CHEMISTRY

Chem.
Elec. Engr.
Meteor.
Phy.

Several efforts are included. AIR-SURFACE EXCHANGE studies use micrometeorological methods with specialized sensors and analysis techniques to measure the tubulent transfer rates of trace substances in the lower atmosphere above natural surfaces. Substances include moisture, carbon dioxide, sulfur and nitrogen compounds, ozone, oxygenated hydrocarbons, and particulate matter. Results are interpreted for use in both site-specific and large-scale modeling. WET DEPOSITION studies center on obtaining important meteorological and chemical information on processes of deposition from the atmosphere in snow and rain, i.e., on wet deposition. Analyses consider the total deposition of sulfur and nitrogen compounds, selected organic species, and particles. REMOTE-PROBING studies use Doppler acoustic remote sensing, UHF radars, and balloon-borne instrumentation to evalute the transport and dispersive properties of the lower atmosphere and to measure the state of the lower atmosphere in support of investigations of global climate change. Analytical and theoretical studies are performed to interpret the data acquired. NUMERICAL MODELING studies emphasize cloud physics, especially the interactions between water vapor, cloud water, and rain or snow. This work is applied to investigations of global climate change.

264 AQUATIC PROCESSES

Appl. Comp.
Envr. Sci.
Phy.

A variety of techniques are used to study contaminant transport and exchange process in the Great Lakes, including *in situ* observations of the benthic boundary layer, numerical modeling, and statistical analysis of water quality data. Procedures such as optimization and inverse analysis are used as well. Equipment used includes current meters, transmissometers, time-lapse cameras, and computers.

265 ENVIRONMENTAL ORGANIC CHEMISTRY

Chem.
Envr. Sci.
Meteor.

The tropospheric chemistry, sources, and transport of both natural and fossil-fuel-derived organic substances are studied in the field and laboratory, with special emphasis on the interactions of organic oxidants, organic nitrates, and precursor aldehydes with energy-related inorganic pollutants (e.g., NO_x, SO_2). Additional studies examine the effects of alcohol fuel usage and the potential impacts of organic tropospheric chemistry on cloud chemistry and physics. The potential role of organic trace species as greenhouse gases is also being explored. State-of-the-art instrumentation for sampling and real-time analysis is used.

TERRESTRIAL SECTION

Research activities conducted in this area involve both field and laboratory investigations on the transport, fate, and biogeochemical behavior of hazardous wastes, including radionuclides. Other studies address the effects of environmental stresses on terrestrial ecosystems, both natural and managed. Environmental stresses include such things as air pollutants, acidic rain, and ozone. Disturbance effects studies examine changes to ecosystems resulting from stresses associated with energy production and use.

266 SUBSURFACE SCIENCE

Bot.
Ecol.
Field Bio.

Subsurface contamination of groundwaters by mixed waste is becoming an increasing environmental concern. Basic research efforts are examining the interactions between radioactive and inorganic contaminants with organic waste in aqueous systems with state-of-the-art spectroscopic techniques. The role of colloids in transporting hydrophobic and hydrophilic pollutants in subsurface groundwaters is being examined by using hollow-fiber ultrafiltration methods. Of particular interest are the interactions of mixed wastes with naturally occuring organic materials (i.e., humic and fulvic acids). These projects, which are part of the Department of Energy's Subsurface Science Program, are developing a better fundamental understanding of the mechanisms and processes involved in groundwater/contaminant/reservoir interactions.

267 TERRESTRIAL ECOLOGY

Bot.
Ecol.
Envr. Sci.
Field Bio.
Micro-bio.

The significance of symbiotic mycorrhizal fungi in the long-term survival of host plants has not been well documented. Research is being conducted on the influence of mycorrhizal fungi on host and nonhost plant survival as it relates to ecosystem recovery, especially as to how this association affects the fitness of the host, both directly and indirectly. In other studies, plant-soil interactions are investigated from the standpoint of the plant-soil interface in a range of systems from row crops to native tallgrass prairie. Field and laboratory studies are conducted to determine the interrelationships between plant roots, associated symbiotic microflora, developing soil structure, and ion and water availability.

268 MICROBIOLOGY

Bio.
Bio-chem.
Bio-tech.
Micro-bio.
Molec. Bio.

Currently, the focus of the microbiology and molecular biology effort is twofold. One project involves the development of stable, high-performance strains of lactic acid bacteria. These strains will be used in a process that transforms high-carbohydrate food waste to bio- and photodegradable plastics. This process has large potential energy savings, helps to solve a wastestream problem for food processors, and is economically attractive; i.e., it leads to preparation of environmentally safe plastics from low-cost biomass. A second project develops fungal, yeast, and bacterial strains and/or consortia for inactivating aromatic and substituted aromatic compounds. Both direct enzyme (ligninase, parathionase, etc.) and microbial (recombinant and nonrecombinant cell) treatments. are being examined for their ability to hydrolyze recalcitrant, xenobiotic (man-made) compounds that can often contaminate soils and groundwaters.

ENVIRONMENTAL PROGRAMS

269 ENVIRONMENTAL MANAGEMENT AND SURVEYS

Comp. Sci.
Envr. Asses.
Field Bio.

This program provides specialized environmental services to the Department of Energy and other federal agencies. These services are in the categories of (1) environmental management (including the design of legally defensible environmental programs that meet statutory requirements) and environmental counseling and (2) environmental audits and surveys that will identify and evaluate environmental problems at specific facilities. Field sampling activities and laboratory analysis are also managed at federally owned locations. Specific activities include the following: (1) designing program elements to carry out quality environmental investigations of federally owned facilities; (2) counseling and training for federal agencies or federally managed facilities on methods and procedures for environmental audits and surveys, field sampling, quality assurance, and environmental compliance issues; (3) conducting environmental audits and surveys (e.g., air pollution, surface and groundwater contamination, and hazardous waste investigations) at specific federal facilities; (4) sampling of air, surface and groundwater, and soil for organic, inorganic, and radiological contamination; (5) analysis of site-specific environmental data in terms of magnitude of problems and in support of proposed remedial actions; (6) developing site assessment methodologies; and (7) facilitating environmental management strategies by the use of computer-based support tools that exploit recent technology in expert systems, relational databases, and geographic information systems. These automated, integrated systems maximize access to available environmental information and knowledge through a user interface.

270 PHOTOPHYSICS AND PHOTOCHEMISTRY

Chem.

Phy.

Research in the laser photophysics and photochemistry program is directed at understanding the formation and subsequent transformation of excited states of atoms and molecules. This program aims at developing new levels of specificity and sensitivity in producing and detecting atoms and molecules at the quantum-state-specific level with special emphasis on understanding the physics and chemistry of excited states. One of the essential and challenging aspects of this program is the effective incorporation of state-of-the-art laser and detection technologies in a rapidly advancing research field. The techniques used in this work are resonantly enhanced multiphoton ionization combined with ion mass analysis, electron kinetic energy analysis, and fluorescent radiation analysis. Most studies involve double resonance excitation; i.e., a tunable "pump" laser is used to excite a target molecule to an intermediate resonant level, and a second, independently tunable "probe" laser is used to probe the various physical and chemical transformations of the excited states, e.g., intramolecular energy redistribution, unimolecular decomposition, collisional energy transfer, reaction cross sections, radioactive decay, and photoabsorption and photoionization of excited states.

271 RADIATION PHYSICS

Comp. Sci.

Phy.

These theoretical studies focus on the elementary interactions of ionizing radiation with matter, considered at the atomic and molecular levels. Investigations include analysis of the penetration of charged particles in matter and of its consequences on matter. Methods are theoretical but often involve critique and the use of much experimental data. Experimental studies address the mechanisms by which electrons deposit energy in collisions with atomic and molecular gases. Activities include (1) analysis of electron energy loss spectra, (2) studies of electronic transition probabilities, (3) mass spectrometric analysis of dissociation products, and (4) application of data to problems of environmental concern.

EXPERIMENTAL BREEDER REACTOR-II (EBR-II)

The EBR-II conducts a developmental program for the liquid-metal-cooled fast neutron breeder reactor. Experimental Breeder Reactor II (located at Argonne-West, near Idaho Falls) is the U.S. Department of Energy's prime facility for irradiation of fuels and materials in the nation's fast-breeder program. Members of the EBR-II project are located at both Argonne-East (Illinois) and Argonne-West (Idaho).

272 DEVELOPMENT OF NEW COMPONENTS AND EXPERIMENTS

Chem. Engr.
Elec. Engr.
Mech. Engr.

The EBR-II Engineering activities at Argonne East (Illinois) deal mainly with the engineering aspects of reactor components and with facilities for experimental irradiations of fuel and structural materials inside the reactor core. Projects include the thermal-hydraulic analysis of advanced subassemblies, experimental determination of flowrates and pressure drops in these subassemblies, joining of materials, for instrumentation, and other analytical or experimental research associated with developing new components for the reactor.

273 REACTOR CONTROL AND TRANSIENT TESTING

Comp. Sci.
Elec. Engr.
Math.
Mech. Engr.
Nucl. Engr.

EBR-II Analysis activities in Illinois include thermalhydraulics, physics, and mechanical analyses in support of plant operation and test program implementation. Of major importance here is developing control strategies and reactor tests to demonstrate innovative concepts for LMR's. The project usually involves computer simulation and plant automation required for testing. The project provides a well rounded description of the phenomena that are important to the dynamic behavior of the developmental LMR's. Most importantly the work is done in close contact with the EBR-II organization developing advanced safety and operation strategies for next-generation LMR power plants. See also Argonne-West for description of projects involving EBR-II and the IFR activities in Idaho.

274 COMPUTER APPLICATIONS DEVELOPMENT

Comp. Sci.
Math.
Nucl. Engr.

Large volumes of digitized data from nuclear reactor experiments are processed, analyzed, and interpreted using state-of-the-art interactive techniques on mainframes and on distributed PCs. Software packages for various numerical, statistical, and time-series analyses are developed, modified, and maintained using a variety of languages and software-engineering tools. On-line expert systems are being developed that use automated reasoning techniques for assistance with the tasks of surveillance, diagnosis, and interpretation of physical parameters in advanced nuclear-reactor subsystems.

FUSION POWER PROGRAM (FPP)

This Program is a multidiscipline activity involving several ANL Scientific and Engineering Divisions which is devoted to the development of magnetic fusion energy and associated advanced fusion reactor technologies. Programs are underway to develop materials and components for reactor first wall, blankets and shields. A wide variety of fusion reactor systems and design studies are carried out.

275 REACTOR SYSTEMS STUDIES

Chem. Engr.
Comp. Sci.
Elec. Engr.

This program is concerned with analyses and comparisons of the relative technical, environmental, and economic merits of various fusion reactor systems. The performance of a fusion power plant is simulated by mathematical models in a computer program. Parametric and sensitivity studies are made to evaluate the severity of various scientific and engineering problems, as well as define the most promising options for technically sound and economically competitive fusion power plants. Current emphasis is on tokamak power reactors.

Envr. Sci.   Math.   Mech. Engr.   Metal Engr.   Nucl. Engr.   Phy.

276 BLANKET AND SHIELD STUDIES

Chem.
Chem. Engr.
Mat. Sci.

This activity is concerned with a general design evaluation of blanket/shield components of fusion reactors. Various combinations of blanket structural material/coolant/tritium breeding material are being reviewed to develop a well-defined set of design criteria. Experimental and analytical activities on first wall/blanket/shield components are underway to develop design tools for reactor first wall, blanket and shield including neutronics, thermal hydraulics, and structural mechanics.

Mech. Engr.   Metal. Engr.   Nucl. Engr.

277 PLASMA ENGINEERING STUDIES

Comp. Sci.
Elec. Engr.

A variety of studies are underway to develop physics models and computer codes to study simulated reactor conditions in magnetic fusion devices. Current emphasis is on plasma impurity control in tokamak devices, plasma heating and current drive using RF technology, reactor startup, and shutdown, and overall power balance and operating conditions.

Math.   Nucl. Engr.   Phy.

7 GeV ADVANCED PHOTON SOURCE PROJECT

This Project is the Laboratory's largest and most important new activity. Currently in progress is pre-construction research and development and construction of the synchrotron facility that will be capable of producing high-intensity, tunable x-ray beams. These photon beams will serve the research needs of many fields of science, including physics, chemistry, materials and surface science, biology and medicine. The accelerator complex under construction consists of a 200 MeV electron linear accelerator, a positron production target, an injector synchrotron to accelerate 450 MeV positrons to 7 GeV, and a 7 GeV positron storage ring of 1104 m circumference with 34 insertion device (undulators and wigglers) beam lines and 35 or more bending magnet beam lines.

278 ACCELERATOR RESEARCH AND DEVELOPMENT

Comp. Sci. *Elec. Engr.*

Current research activities include accelerator physics research, charged-particle beam dynamics calculations, particle beam transport design, prototype construction and measurement of accelerator magnets, fabrication and testing of vacuum system prototypes, radio-frequency acceleration system measurements, accelerator diagnostic system research and development, and computer-based accelerator control system.

Mat. Sci. *Mech. Engr.* *Phy.*

279 INSERTION DEVICES, X-RAY OPTICS, AND DETECTOR DEVELOPMENT

Bio. *Chem.*

These activities include research and development on instrumentation needed for the Experimental Facilities area of the Advanced Photon Source. Current activities involve prototyping efforts related to insertion devices, beam line components, x-ray optics, detectors, novel synchrotron instrumentation, and other user equipment.

Mat. Sci. *Metal. Engr.* *Phy.*

280 FACILITIES CONSTRUCTION AND PROJECT MANAGEMENT

Civil Engr. *Elec. Engr.*

These activities include construction-related field engineering, safety and environmental engineering, cost and schedule analysis and control, quality assurance and project management support. Initial construction of the facilities will also involve field engineering management, civil engineering, and site preparation work

Mech. Engr. *Constr. Mngmt.*

HIGH ENERGY PHYSICS DIVISION (HEP)

This Division conducts research into the nature and properties of elementary particles -- the building blocks of matter. The program includes colliding beam experiments at the proton-antiproton collider (TEV-I) at nearby Fermi National Accelerator Laboratory. A calorimetric detector is being built for the HERA electron-proton collider in Hamburg, West Germany. The effects of spin in elementary particle scattering are being studied over a wide range of energies. Research not requiring particle accelerators includes construction of a major underground detector to search for proton decay and the use of superspeed multinode processors for lattice gauge computations. The Division's theoretical group is active in several areas of elementary particle theory. Accelerator physics research includes development of new acceleration techniques and designs for new accelerator facilities.

281 LEPTON SCATTERING EXPERIMENTS

Engr.
Phy.

At the DESY Laboratory in Hamburg, West Germany, an electron-proton storage ring system is under construction that will collide 30 GeV electrons with 820 GeV protons. The Argonne group, together with physicists from six U.S. universities, is working in an International Collaboration to design, build, and operate a large spectrometer called ZEUS to study electron-proton collisions at this facility. The U.S. responsibility on the detector is the barrel calorimeter which consists of sets of 119 thin plates of depleted uranium sandwiched with plates of scintillator. Thirty-two, wedge-shaped modules fit together to form a 6 m diameter barrel. The light pulses resulting from interactions of the particles absorbed in the calorimeter are recorded by about 5000 photomultiplier tubes. Through a compensation mechanism, the energy resolution for hadrons will be superior to any achieved to date. The construction of the modules will be completed early in 1991. An extensive program to study the performance of these calorimeters and the stability of their calibration is being carried out, both using cosmic rays and a test beam facility. The first ep collisions in ZEUS will occur in the summer of 1991. There are opportunities for both faculty and students to become involved in data analysis, hardware construction, and hardware testing.

282 NUCLEON DECAY EXPERIMENT

Engr.
Phy.

Unified theories of elementary particle interactions indicate that the decay of nucleons (protons and bound neutrons) may occur at an observable rate close to the present experimental limits. The observation of nucleon decay would profoundly influence our view of the physical world, and it would dramatically establish a unification among the strong, electromagnetic, and weak interactions. The so-called Grand Unified Theories can also explain the observed predominance of matter over antimatter in the universe and predict the existence of magnetic monopoles.

Physicists from Argonne's High Energy Physics Division, the University of Minnesota, Oxford University, the Rutherford Laboratory, and Tufts University are building a 1000-ton tracking calorimeter to search for nucleon instability, sensitive to lifetimes as long as 10^{32} years in many different decay modes. The experiment, called Soudan 2, will also be used to search for magnetic monopoles and to study cosmic-ray phenomena with unprecedented sensitivity. The first half of the Soudan 2 detector is now in operation, 2300 feet underground in the Soudan mine. There are opportunities for students and faculty to become involved in several aspects of this project in the High Energy Physics Division, including the analysis of data from Soudan 2 and studies of a 5-ton module performance.

283 EXPERIMENTS USING POLARIZED BEAMS AND TARGETS

Phy. This program consists of several experiments studying the spin dependence of proton-proton and antiproton-proton interactions at high energies. The experiments use both polarized beams and targets, in which the spin of the particles are aligned in certain directions. Polarization experiments in nucleon-nucleon scattering can test predictions made by the QCD (quantum chromodynamics) theory.

These high-energy experiments use a newly-constructed beam line at Fermilab. With a momentum of 200 GeV/c, it is presently the highest energy beam of polarized protons and the only available beam of polarized antiprotons. Two polarimeters were used to confirm the average polarization of the beam. The polarized protons originate from the decays of lambda particles, and are electronically tagged to determine both their momentum and polarization values. Current experiments include measurements of $\Delta\sigma_L$ (the difference in total cross section for longitudinal spin states), the large transverse momentum production of neutral pions, and the large-X_F production of $\pi^{\pm}$, π°, Λ, and Σ particles for both p-p and p-p interactions.

284 PROTON-ANTIPROTON COLLIDER EXPERIMENTS

Phy. This activity is part of an international collaborative effort to study proton-antiproton collisions using the Collider Detector at Fermilab. The 1800 GeV center-of-mass collision energy is the highest currently available in particle physics, and has opened up new possibilities for studying phenomena. The detector contains a large solenoidal magnet with extensive charged-particle tracking devices, completely surrounded by calorimeters. The electromagnetic calorimeter design and construction was led by the Argonne group. Almost 5 pb^{-1} of integrated luminosity has been obtained running at the Tevatron Collider. This sample has been used to make precision measurements of the W and Z gauge boson masses, and to set stringent new limits on the mass of the long-awaited "top" quark. In addition this data set is being used for detailed studies of QCD production of heavy quarks (bottom and charm) and direct photons. Argonne is responsible for an upgrade of the central calorimetry that will provide better electron and prompt photon identification for the 1991 run, which is expected to give a five-times larger event sample.

The Argonne group is involved with the construction of various particle detectors, such as multiwire proportional chambers, the construction of the polarized proton target for these experiments, and the analysis of the data. Argonne leads an international collaboration consisting of groups from Saclay (France), Fermilab, Serpukhov (USSR), Kyoto (Japan), LAPP (France), Los Alamos, Northwestern, Rice, Japan, and Trieste (Italy), Udine (Italy).

285 ACCELERATOR PHYSICS GROUP

Elec. Engr.

Experimental and theoretical studies are underway to develop novel techniques for particle acceleration. Such techniques will be required to enable future exploration of physics at the highest energies. An R&D facility, constructed at the Argonne 22-MeV linear accelerator, enables measurement of high gradient electric fields using very short pulses of relativistic electrons. These fields are obtained as wake fields generated by precisely-timed, high-current pulses from the same linear accelerator serving as lead or driver pulses. The facility is being used to perform experiments on a wide variety of acceleration techniques using plasmas and passive structures.

A new, more powerful wake field test facility is now under construction. This new project includes a high current laser photocathode electron gun, and a 150-MeV RF linac which drives a dielectric wake field accelerator. Accelerating gradients of 100-300 MeV/m can be studied and demonstrated with the new facility. A goal is to construct a 1 GeV demonstration accelerator based on wake field technology.

A wide variety of areas are relevant to this project, including laser and particle beam physics, microwave dielectric properties of materials, RF cavity and magnet design, and accelerator theory and simulation. The simulation effort includes the development of accelerator physics codes on the parallel computers available at Argonne.

286 SSC DETECTOR R&D

Comp. Sci.

Elec. Engr.

Mat. Sci.

Phy.

The Superconducting Super Collider (SSC) is the next generation high energy physics accelerator. This machine will allow observation of collisions at energies more than an order of magnitude higher than are attainable at present facilities. The energy has been chosen to be high enough that the new phenomena which are needed to complete the present standard model of particle interactions must begin to reveal themselves. The high energy and high intensity of the SSC, however, create an experimental climate much more severe than at present machines. Substantial new R&D is needed into new experimental techniques for use at the SSC. In many cases, discovery of the new physics reactions that may occur would be impossible with present apparatus. Three projects are underway now and others may be started. The present projects are: (a) software for simulation of detectors needed because of the great complexity and precision demanded of detectors at the SSC; (b) radiation-hard VLSI readout electronics to withstand the unprecedented radiation fields that will be encountered at the SSC; and (c) simulation, design and prototyping of a scintillator-based calorimeter for use in an SSC detector. A wide variety of disciplines are involved in these projects, including computer science and materials science, in addition to physics. Data from these projects will be used in preparation of a proposal for an SSC experiment.

INTENSE PULSED NEUTRON SOURCE DIVISION (IPNS)

The Intense Pulsed Neutron Source Division (IPNS) is an accelerator-based source of neutrons for basic research in condensed matter using neutron scattering techniques. The IPNS program is operated in a user-oriented mode with eleven neutron scattering instruments. Research using these facilities is sponsored by various research divisions.

287 IPNS DATA ACQUISITION SYSTEMS

Bio.
Chem.
Comp. Sci.
Elec. Engr.
Mat. Sci.
Phy.

The IPNS Data acquisition system consists of PDP-11, microVAX and VAX computer systems, plus dedicated microprocessors for data collection and storage. The PDP-11 sets up and controls the functions of the microprocessor, displays and stores the data, controls the experiment, and communicates with the user and the VAX computer through DECNET/Ethernet. The VAX systems receive data from the PDP-11's and are used for data concentration, analysis, and storage. We are in the process of modifying our data collection software to run on a micro-VAX computer instead of a PDP-11. We are also in the process of developing graphics software using the Graphics Kernel System (GKS) to make our complete analysis codes transportable. Research participants would assist in development of code or characteriziation of equipment for experimental control (temperature, position, etc.) or for data collection, analysis, and display on a VAX or micro VAX using FORTRAN and GKS. Major equipment includes: VAX 11/750, seven PDP 11's, five micro VAX's and numerous Z-8001's microprocessors.

288 IPNS ACCELERATOR SYSTEM

Elec. Engr.
Mech. Engr.
Phy.

The IPNS accelerator system is an operating facility consisting of an H^- ion source, a 750 keV Cockcroft-Walton dc preaccelerator, a 50 MeV Alvarez linac and a 500 MeV Rapid Cycling Synchrotron. Particle accelerator technology features high current regulated magnet power supplies; frequency, amplitude and phase modulated high power rf transmitters; vacuum systems; analog and digital control and feedback circuits; and dedicated computer control systems. Improvements and modifications to various systems and investigation of beam performance is continually ongoing providing the participants with a unique experience in the physics of charged-particle dynamics, as well as, a wide variety of engineering specialities.

289 IPNS NEUTRON PHYSICS

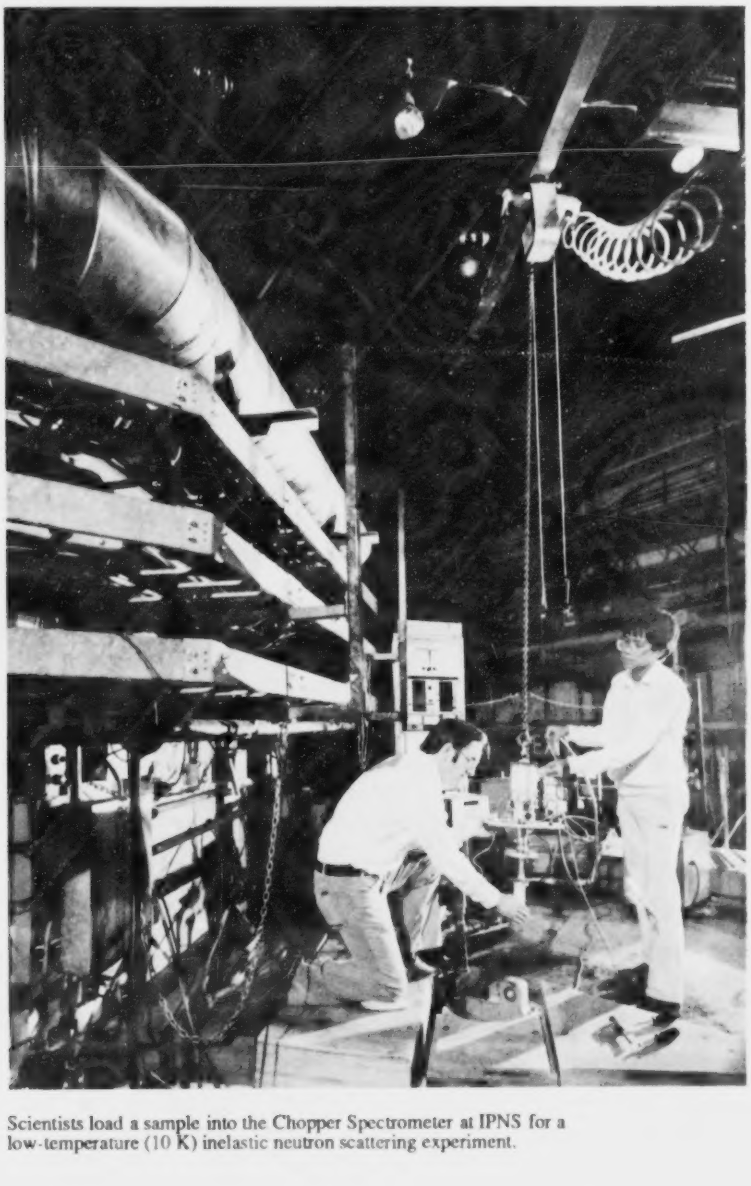
Mat. Sci.
Nucl. Engr.

The IPNS neutron generating system consists of an enriched uranium target surrounded by liquid and solid methane (CH_4) and liquid hydrogen (H_2) moderators for slowing the neutrons down to energies appropriate for neutron scattering studies. Participants will assist senior staff on a variety of measurements to characterize target, moderator and instrument performance. Target/moderator programs include measurements on pulse shape, neutron spectra, energy deposition, and radiation damage in the moderators; and energy deposition, delayed neutrons and shielding of the uranium target. Instrument programs include the design, testing, or characterization of components or systems for neutron detection, shielding and background reduction, and neutron optics in neutron scattering instruments.

290 IPNS NEUTRON SCATTERING RESEARCH

Bio. *Chem.* *Mat. Sci.* *Phy.*

The IPNS neutron scattering facility consists of 11 instruments for investigating the structural and dynamical properties of condensed matter. The neutron scattering instruments are diffractometers (powder, single crystal and small angle), spectrometers (for investigating energy transfers from 50 μeV to 1.5 meV) and reflectometers. Over 300 experiments are performed per year in various areas of materials science, physics, chemistry, biology and applied technology. Recent studies include the structure of high temperature superconductors, interdiffusion of polymers, formation and structure of zeolites, intermediates range order in glasses, residual stresses in composities and magnetic excitations in actinide compounds.



Scientists load a sample into the Chopper Spectrometer at IPNS for a low-temperature (10 K) inelastic neutron scattering experiment.

MATERIALS AND COMPONENTS TECHNOLOGY DIVISION (MCT)

The Materials and Components Technology Division (MCT) provides an integrated, state-of-the-art approach to the design, fabrication, and testing of highly reliable materials, components, and instrumentation. The Division is particularly strong in the areas of high-temperature properties of metals and ceramics, corrosion, radiation effects, nondestructive evaluation techniques, materials processing, thermal hydraulics, engineering mechanics, instrumentation and control, and components and systems testing. For energy technologies, the Division's programs emphasize safe and reliable design, efficient performance, and inherent safety of components and systems, as well as gathering basic engineering data and developing applicable new methods of analysis.

291 INSTRUMENTATION AND NONDESTRUCTIVE EVALUATION

Chem. Engr.
Comp. Sci.
Elec. Engr.

Recent advances in sensor/instrumentation technology, aimed at the development of nonintrusive devices for process control or diagnostics, have created many parallels with the techniques used for nondestructive evaluation (NDE) of materials. Techniques based on wave propagation are used both to sense parameters and to evaluate materials. In addition, the signal-processing mechanisms and requirements for both areas are identical. By bringing instrumentation and NDE efforts together under a common umbrella, MCT has greatly enhanced its capabilities in both areas.

Engr. Phy.
Mech. Engr.
Nucl. Engr.

The current instrumentation efforts of the Section focus on the development of advanced sensors and process control systems in support of DOE's Fossil and Nuclear Energy Research. This work encompasses (a) multiphase flow measurement techniques, including in-situ measurement of temperature, fluid level, pressure, density, and viscosity; (b) millimeter wave diagnostics for coal conversion systems; (c) leak detection systems; (d) control schemes for future process plants; (e) acoustic/ultrasonic surveillance of nuclear power plants; (f) neutron detectors for nuclear power plants; (g) Btu meters for district heating and cooling; and (h) process development for electromagnetic continuous casting of steel.

Phy.

Our NDE efforts focus on development of techniques and systems for materials characterization and evaluation of component reliability. This work includes (a) characterizing materials, especially ceramics, during various stages of fabrication; (b) evaluating the structural integrity of components of a wide variety of energy systems; (c) pinpointing causes and remedies for improper component behavior through failure analyses; (d) establishing deterioration rates of materials (especially stone) exposed to acid rain; (e) developing low-frequency transducers for the inspection of concrete; and (f) developing on-line viscosity and erosion monitoring systems for fossil energy plants.

292 SYSTEMS AND COMPONENTS

Mech. Engr.
Nucl. Engr.
Elec. Engr.

This group is involved in conducting applied research and exploratory development as related to advanced energy systems and components. It is focused on both nuclear and nonnuclear systems and components. In the nuclear area, effort is directed at the Integral Fast Reactor (IFR) Fuel Cycle, Electromagnetic Pumps, and Steam Generators. In the nonnuclear area, research and development effort is directed at Heat Pipes, Stirling Cycles, Organic Rankine Cycles, High-T_c Superconductivity, Magnetic Refrigeration, Electromagnetic Pumps, and Thermal Decomposition of Fuels. Both analytical and experimental research is being conducted within the group, with major efforts in the area of the IFR Fuel Cycle, and Electromagnetic Pumps.

293 ANALYTICAL THERMAL HYDRAULIC RESEARCH PROGRAM

Chem. Engr.
Comp. Sci.
Math.
Mech. Engr.
Nucl. Engr.
Phy.

The Analytical Thermal Hydraulic Research Program is responsible for mathematical modeling of thermal-hydraulic physical phenomena and for developing computer codes (COMMIX and BODYFIT series) that can analyze heat transfer and fluid flow conditions in components of various engineering systems. The computer codes being developed are single-phase/multiphase conservation equations of mass, momentum, and energy. The COMMIX series uses volume porosity surface permeability, distributed resistance, and distributed heat source concepts to analyze continuum/quasi-continuum flow domains. The BODYFIT series uses boundary fitted coordinate transformation approach to analyze continuum quasi-continuum flow domains. The COMMIX and BODYFIT series have a wide range of applicability and have been successfully used to analyze (1) reactor fuel assemblies (rod bundles), (2) reactor plenum mixing problems, (3) flow stratification problems in a pipe, (4) reactor heat exchangers, (5) reactor steam generators, (6) thermocline storage tanks for solar applications, (7) fluidized bed combustion processes, (8) rock beds, (9) solar ponds, and (10) piping systems and valves. The program also involves operation of the 43 m x 25 m x 4.2 m deep ANL Research Salt Gradient Solar Pond and studying various thermohydrodynamic phenomena related to it.

294 MECHANICS AND VIBRATIONS

Appl. Math.
Appl. Mech.
Civil Engr.
Comp. Sci.
Mech. Engr.

Research in this group relates to many diverse areas of structural dynamics, fluid mechanics, and vibrations. Primary applications involve the determination of loads and structural response in advanced energy systems. The current scope of the Section's activities includes investigations on vibrations, seismic studies for light-water reactors (LWRs) and New Production Reactor (NPR) concepts, support efforts for liquid metal-cooled reactors (LMRs), computational fluid mechanics, and basic studies in mechanics. A continuing effort is in progress to develop/improve analysis, test methods and data bases in flow-induced vibrations for applications to nuclear power plant components and systems, heat exchangers and flow systems. Other current studies emphasize two-phase flows in heat exchangers and the heat transfer of nonazeotropic mixtures. A specific vibration study concerns the characterization of vibration sources and response of the 7 GeV Synchrotron radiation research facility to be built at Argonne. There is a continuing effort to validate seismic calculational methods used in the design and risk assessment of nuclear power plants. This involves the participation in the design and execution of vibration and seismic experiments on large/full-scale structures at overseas facilities. To support the design of advanced LMRs, sodium-water reaction studies are performed using the Argonne developed SWAAM codes. Similarly the Argonne developed COMMIX-1AR code is used to perform thermal hydraulic analyses under normal and off-normal reactor operating conditions. Other design activities include the thermal and structural analysis of reactor components, the development of seismic isolation concepts and the seismic qualification of equipment. The basic mechanics studies include the development of load correlation parameters for bounding the dynamic plastic deformation of structures, an integrated theoretical/experimental study of nonlinear stability phenomena involving both fluids and structures and their coupling, and an investigation of structural damage assessment from changes in dynamic characteristics. The group also performs experimental and analytical studies related to industrial applications of high-temperature superconductors. These include evaluating the stability of magnetically levitated bearings and the dynamic response of magnetically levitated vehicles.

295 SALT GRADIENT SOLAR POND RESEARCH

Chem. Engr.
Comp. Sci.
Mech. Engr.
Phy. Engr.

Salt gradient solar ponds provide low-temperature (below 100°C) energy for heating and power generation. Theoretical research in this area includes analytical studies related to fundamental phenomena (double-diffusive convection) and computer modeling of instabilities in the salt gradient, surface disturbances, and pond bottom reflectivity control. Experimental research includes measurement of temperature and salinity in the pond, ground temperatures, and solar insolation. Test instrumentation is supported by micro- and mini-computer based systems.

296 TRANSPORTATION OF HAZARDOUS MATERIALS

Appl. Math.
Chem. Engr.
Civil Engr.
Comp. Sci.
Mech. Engr.
Nucl. Engr.
Phy.
Traf. Mgmt.

This group provides technical assistance to the Department of Energy (DOE) by addressing department-wide transportation, traffic management, and waste management options. Generic national and international issues are considered, including packaging certification, transportation tracking systems, related regulations and legislation, and waste repository configurations. Examples of the tasks include the development of an intelligent terminal data base system for retrieving microfilmed transportation legal-brief documents, the review and analysis of DOE-generated reports, and the technical review of Safety Analysis Reports for Packaging (SARPs). These SARP reviews involve general information and drawings, structural, thermal, containment, shielding, critically operating procedures, acceptance tests and maintenance programs, and quality assurance. Computer codes are used for analyses.

297 CERAMICS

Ceram. Engr.
Mat. Sci.

Ceramic processing development and new ceramic materials synthesis for a wide variety of applications are carried out in this section. Much of the work is done on a collaborative basis with other groups both within and outside of Argonne. An example is the conductor development using high-T_C ceramic superconductors. The Ceramics Section staff have fabricated wires and other technologically useful shapes for motors, bearings, sensors, etc. as well as synthesized new superconducting compounds. Other areas include ceramic matrix-ceramic fiber composites which are being studied for a variety of high-temperature applications, ionic conductors for batteries and fuel cells, and advanced refractories for iron and steel making and for the reduction of nuclear waste. Generally, in the Ceramics Section work, includes microstructural characterization by optical and electron microscopy, mechanical properties measurement, and, for the superconductors, determination of critical current density and critical temperature. For composites, we are using neutron diffraction to characterize the internal stress distribution. Those interested in hands-on ceramics laboratory work should apply for a position in this section.

298 MECHANICAL PROPERTIES OF METALS

Comp. Sci.
Mat. Sci.
Mech. Engr.
Metal. Engr.

This section is involved in the study of mechanical behavior of structural alloys used in a number of energy systems. Group research activities include: (1) the stress corrosion cracking, fatigue, and crack growth behaviors of austenitic and ferritic steels in water-cooled nuclear reactor environments, (2) the cracking resistance of candidate alloys for nuclear waste containment, (3) microstructural analysis and mechanical properties determinations for nuclear pressure vessel alloys subjected to accident conditions, (4) computer analyses of structural components and tritium breeding materials for fusion reactor applications, (5) the analysis of nuclear fuel behavior under off-normal and accident conditions, and (6) failure analysis of actual components from nuclear power plants and other energy systems. Some projects involve laboratory testing of specimens under operating temperatures and pressures, while others rely on computer analyses to determine the expected materials behavior. This section offers the candidate the opportunity to work on real-world materials problems utilizing advanced mechanical testing equipment and environmental control systems, sophisticated microstructural characterization instrumentation (scanning and Auger electron microscopes and the electron microprobe), and advanced computer systems and software.

299 ANALYSIS AND MODELING OF MATERIALS BEHAVIOR IN ENERGY SYSTEMS

Comp. Sci.
Math.
Mech. Engr.
Metal. Engr.
Nucl. Engr.

A modern, high-speed, digital computer is employed to simulate the physical behavior of materials used in advanced energy systems (fission and fusion). In the fission area, the thermal, mechanical and irradiation response of fuel elements in light water reactors and in liquid-metal fast breeder reactors (LMFBRs) is analyzed. Two computer-based codes are under development. Emphasis is placed on realistic models that accurately describe the physical situation. The LIFE-4 code has been designed to calculate the behavior of LMFBR fuel elements consisting of (U, Pu)O_2 driver or UO blanket fuels, stainless steel or advanced alloy claddings, and liquid sodium coolant. Code development emphasis has been on operational transient fuel element performance with modeling of transient gas behavior, high-temperature fuel creep, high-strain-rate cladding deformation and transient failure predictions. The GRASS-SST/FASTGRASS/PARAGRASS code system is being developed in order to assess the behavior of fission products (noble gases, I, Cs, CsI, MoO_4, Cs_2, UO_4) in LWR fuel under normal and accident conditions. In the fusion area, the thermal, mechanical and irradiation performance of solid breeders (Li_2O and other ternary oxides) are being modeled. The effort, recently initiated, is at a rapidly expanding stage with a long-range goal of developing an integrated computer code for performance prediction of fusion solid breeder blankets. Research activities include the analysis of specific phenomena in order to identify key process and/or physical parameters which affect material performance.

300 IRRADIATION PERFORMANCE OF REACTOR MATERIALS

Metal.
Metal. Engr.
Nucl. Engr.
Ceram.

The principal objective of the programs in the Irradiation Performance Section is to determine and assess the behavior of materials, principally fuels and claddings, in the environment of nuclear reactors. This environment results in neutron damage and chemical, metallurgical, and mechanical processes that occur over a wide range of elevated temperatures. The programs fall into two categories: (1) fuel system development for a number of reactor types, and (2) postirradiation characterization of materials from existing reactors. The fuel development activities include planning of experiments for irradiation in a reactor, the postirradiation examination of these experiments, postirradiation testing of materials and components, and the evaluation and analysis of the results. Programs in postirradiation characterization involve examinations, testing and data analysis. Current efforts include fuel development for Argonne's metal-fueled Integral Fast Reactor, oxide-fueled liquid metal-cooled reactors (LMRs), and research and test reactors (based on reduced enrichment fuels). The principal program on characterizing irradiated materials involves materials from the TMI core and vessel, with smaller efforts on other LWR materials problems. The Section operates the Alpha-Gamma Hot Cell Facility (AGHCF), in which primarily fuel elements are examined, and the Irradiated Materials Laboratory (IML), a smaller hot-cell in which the mechanical property testing is performed. Available research tools include optical metallography, SEM, electron microprobe analysis, and scanning Auger microscopy. Cooperative research programs are welcomed.

301 EMBRITTLEMENT OF CAST STAINLESS STEELS IN LIGHT WATER REACTOR SYSTEMS

Mat. Sci.
Metal. Engr.

The program involves an experimental investigation of the loss in toughness suffered by cast components under normal reactor operating conditions. Microstructural changes as well as mechanical properties, such as impact strength, tensile properties, and fracture toughness, are being determined for several long-term aged cast materials to establish the mechanism and the kinetics of low-temperature embrittlement. The research requires some background in the areas of mechanical testing, electron microscopy, and physical metallurgy.

302 OXIDATION-SULFIDATION BEHAVIOR OF MATERIALS

Mat. Sci.
Metal. Engr.

The program involves experimental studies to establish the mechanism of oxidation-sulfidation of model metallic materials exposed to complex and multicomponent gas environments. The research will require background in the areas of thermodynamics and kinetics of gas-solid reactions and use of optical and electron microscopy techniques to elucidate the corrosion mechanisms.

303 CORROSION OF MATERIALS IN THE PRESENCE OF DEPOSITS

Mat. Sci.
Mech. Engr.

The program involves experimental studies to establish the mechanisms of corrosion of heat-exchanger and gas turbine materials in the presence of deposits that are generated during the combustion of coal and coal-derived fuels. The research will require background in the areas of thermodynamics and kinetics of gas-solid reactions and fluid-flow characteristics which influence the type and rate of deposit(s). A background in x-ray diffraction is desirable.

304 COMPATIBILITY OF STRUCTURAL MATERIALS WITH LIQUID LITHIUM

Mat. Sci.
Mech. Engr.
Metal. Engr.

The program involves experimental studies to investigate the influence of chemical environment on the compatibility, corrosion, and mechanical properties of structural materials under conditions of interest in fusion reactors. Test environments include liquid lithium and lithium alloys. The research requires some background in the areas of mechanical testing, thermodynamics, electron microscopy and x-ray diffraction techniques to evaluate the environmental effects.

305 STRESS-CORROSION CRACKING OF LIGHT WATER REACTOR MATERIALS IN SIMULATED COOLANT ENVIRONMENTS

Chem.
Mat. Sci.
Metal Engr.

The program involves an experimental investigation of the influence of simulated reactor-coolant environments, under normal and off-normal water chemistry conditions, on the susceptibility of piping and structural materials to stress-corrosion cracking. The effect of micro-structure of the materials, water chemistry (viz. oxygen, hydrogen and impurity concentrations, pH), and temperature on the rate and mode of crack growth is being determined for a range of loading conditions. Background in the areas of electrochemistry, electron microscopy, aqueous corrosion, and physical metallurgy are applicable.

306 ALLOY MODIFICATION FOR IMPROVED CORROSION RESISTANCE

Mat. Sci.
Metal. Engr.
Surf. Sci.

The program involves experimental studies to establish the composition and microstructure of surface layers (created by ion implantation, surface coating, laser annealing, etc.) that impart improved corrosion resistance in oxygen and oxygen-sulfur-chloride environments. A background in transmission electron microscopy and Auger Electron Spectroscopy is desirable.

307 TRIBOLOGY

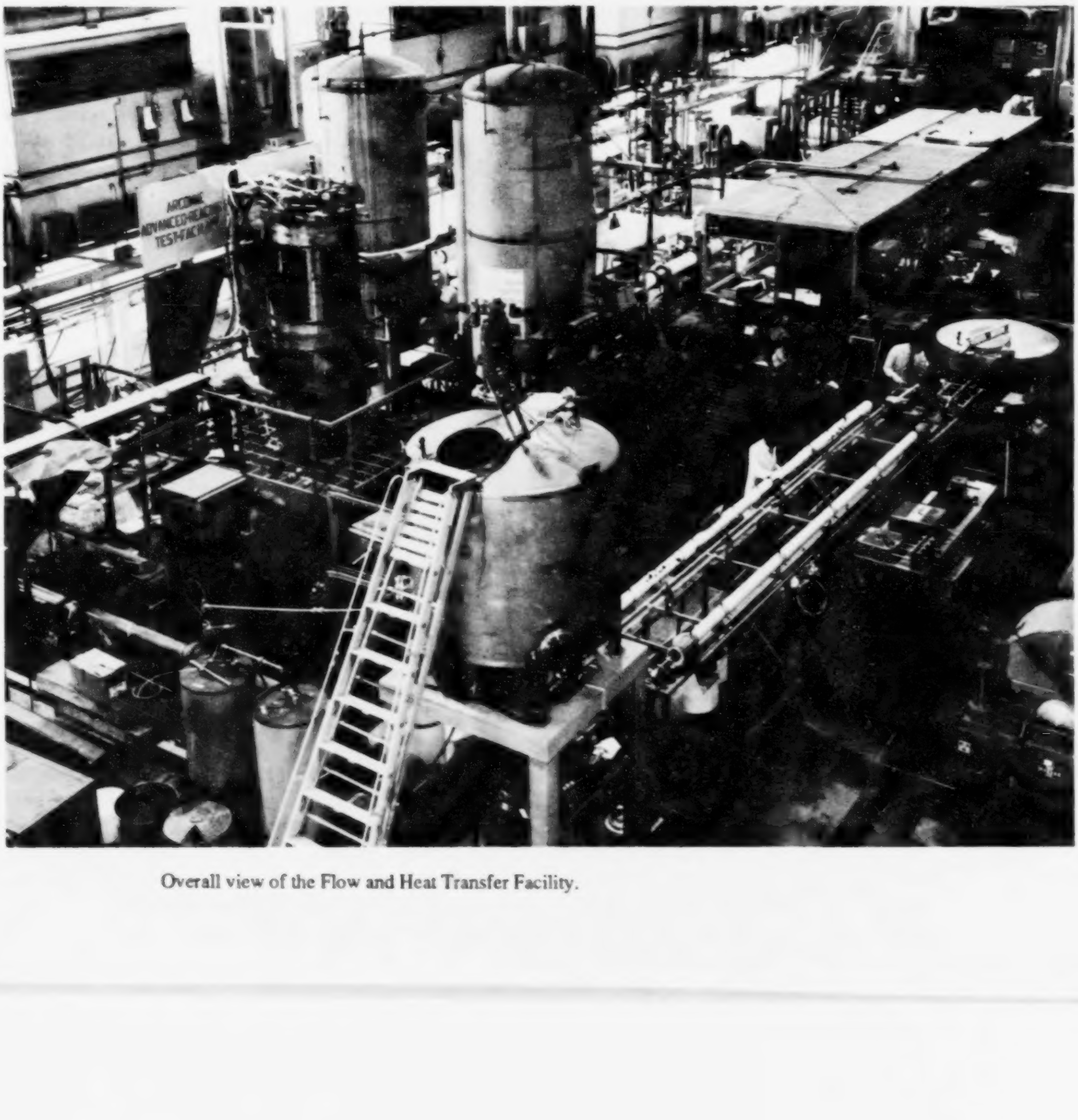
Comp. Sci.
Mat. Sci.
Metal.
Metal. Engr.
Phy.
Surf. Sci.
Tribo. Sci. & Engr.

This section is concerned with the development of materials and surfaces with low coefficients of friction and high wear-resistance, especially for applications involving high temperatures and aggressive chemical atmospheres (e.g., low-heat-rejection engines). The research activities are divided into three areas: (1) characterization and analysis of surfaces and coatings, (2) modification of surface tribological properties by the implantation of ions and the deposition of coatings, (3) friction and wear testing and analysis. The characterization methods include scanning and transmission electron microscopy, scanning Auger microscopy, optical microscopy, X-ray analysis and Rutherford backscattering analysis. A new, JEOL high resolution scanning electron microscope has been acquired. Surface morphology, composition, purity, microstructure, crystal structure and the distribution of implanted ions are determined. Ions are implanted into the surfaces of metals and ceramics to reduce the coefficient of friction and to increase the wear resistance of the surface, or to prepare the surface for the deposition of highly adherent, low-friction, high-wear coatings. Ion beam assisted deposition (simultaneous coating deposition and ion-beam bombardment) as a means to develop highly adherent, low friction and wear surfaces is a major activity. A vacuum chamber containing dual electron beam evaporation sources and ion implanters has been developed and is being utilized in this research. Thermal properties are also a major consideration since these materials are intended primarily for high-temperature applications. A computer modeling effort, to guide the experimental activities, is a strong part of this program. A friction and wear testing and analysis laboratory has recently been set up. A Tally-Surf surface topology measuring system, and high and low frequency oscillatory and unidirectional friction and wear testers for operation under low and high temperature and controlled atmosphere conditions have been acquired and installed. A microwave diamond film, deposition system has been recently acquired.

308 EXPERIMENTAL THERMAL-HYDRAULICS

Mech. Engr.
Chem. Engr.
Nucl. Engr.
Appl. Math.
Comp. Sci.

Research involves experimental thermal-hydraulics as well as phenomenological modeling and analysis related to flow and heat transfer mechanisms associated with single and multiphase flows occurring in advanced energy systems and in the individual components that comprise the systems. The Section operates a unique state-of-the-art Flow and Heat Transfer Test Facility. This facility includes a broad range of test loops for single and multiphase (gas-liquid and solid-liquid) flows, along with equipment for flow, temperature, pressure, and fluid rheology measurements and flow visualization. With this wide spectrum of capabilities and resources, the Section performs fundamental research as well as development and performance testing of thermal system components. The scope of the Section's present activities includes research on advanced liquid metal-cooled and heavy water reactors , district heating and cooling (DHC) energy conservation technology, slurry heat transfer, coal-water slurry (CWS) rheology, erosion/corrosion in light-water reactor piping, heat and mass transfer in food frying, optical path cooling for high-energy beams, boiling in non-newtonian viscoelastic fluids and development of high temperature superconducting magnetic energy storage devices for terrestrial and satelite applications.



Overall view of the Flow and Heat Transfer Facility.

MATERIALS SCIENCE DIVISION (MSD)

This Division conducts basic research on metals, alloys, ceramics - including high Tc superconductors, and glasses that could have applications in advanced energy systems. The research programs are focused on the structure and properties of materials under extreme conditions of temperature, pressure, radiation flux, and chemical environment. The Division is a major user of the Intense Pulsed Neutron Source (IPNS) and synchrotrons, and operates the high-voltage electron microscope-Tandem Accelerator System as a national user facility. The Division consists of three sections: Advanced Materials, Defects and Radiation Effects, Surface Science and Corrosion.

309 TWO-DIMENSIONAL MATERIALS

Chem.
Elec. Engr.
Mat. Sci.
Phy.

This group prepares and characterizes ultrathin films with novel properties. The materials are prepared as surfaces, interfaces, heterostructures, sandwiches, and superlattices using molecular-beam epitaxy and sputtering techniques. Interest focuses on magnetic, superconducting, optical, transport, and elastic properties. Characterization techniques include ultrahigh vacuum electron spectroscopies and diffraction, light scattering (Raman, Brillouin) and the magneto-optic Kerr effect. Participants aid in film preparation, and analysis and modeling of physical properties. Data handling via computer is usually part of the assignment.

310 APPLIED SUPERCONDUCTIVITY

Elec. Engr.
Mat. Sci.
Phy.

Superconducting thin films including high-temperature superconductors are studied for their potential use in various applications such as the large superconducting magnets needed, for example, in magnetically confined fusion. Participants might be involved in low temperature measurements, sophisticated vapor deposition techniques and/or analysis such as x-ray crystallography and electron microscopy.

311 BASIC SUPERCONDUCTIVITY

Chem.
Elec. Engr.
Mat. Sci.
Phy.

Experimental and theoretical investigations are being carried out on the electronic and magnetic properties of a wide class of materials. Experimental techniques include de Haas van Alphen measurements, Mossbauer spectroscopy, transport measurements, electron tunneling studies, magnetization and susceptibility studies, heat capacity measurements, and materials preparation and characterization efforts. Current activities are concerned primarily with high-temperature ceramic superconductors. Participants will be involved with a specific project involving sample preparation and/or the collection and analysis of data, thus learning the fundamentals of particular techniques.

312 NEUTRON SCATTERING

Chem.
Elec. Engr.
Mat. Sci.
Phy.

Neutron scattering experiments are based on time-of-flight diffraction techniques at the Intense Pulsed Neutron Source in conjunction with computer analysis of the data. Available equipment offers a wide variety of high and low temperature and high pressure environments. Structure of high-temperature superconductors, atomic structure and dynamics of polycrystalline and amorphous solids and liquids, magnetic excitations in crystals and molecular vibrational spectra are being pursued. Participants are involved in studies utilizing the instruments on IPNS and analysis using local computational resources (two VAX's and several microVAX's).

313 CONDENSED MATTER THEORY

Chem.
Comp. Sci.
Mat. Sci.
Phy.

A broad range of problems is studied either for intrinsic significance in the theory of condensed matter or direct relevance to current experiments--often within MSD. Methods range from very formal to computer-intensive calculations and simulations. Research centers in three areas: (1) studies in statistical physics using molecular dynamics and Monte Carlo techniques to investigate phase transitions, glasses quasicrystals, clusters, and nanocrystals: (2) Electronic structure and properties of strongly correlated metals, alloys, and the defected solid state; (3) Microscopic and phenomenological theories of superconductivity. Projects appropriate to participants often involve some computation so knowledge of a computer language (FORTRAN or C) is valuable.

314 BASIC CERAMICS

Ceram.
Chem.
Mat. Sci.
Phy.

This multidisciplinary program, involving a wide variety of theoretical and experimental techniques, is designed to assess the nature of bonding of metal ions, vacancies and defect complexes in oxides of different structure types and the various factors affecting the phase stability and various properties of these complex oxides. Electronic and atomic structure, phase stability and transport in bulk and thin film multicomponent (including high Tc superconducting) oxides are being investigated theoretically, by means of first principle quantum mechanical calculations, and experimentally, using x-ray absorption spectroscopy, x-ray photoelecton spectroscopy, electrical conductivity and optical spectroscopy techniques. Lattice properties and dynamics are being studied experimentally using x-ray diffraction, ultrasonic velocity, heat capacity, Raman and Brillouin scattering measurements. A coordinated experimental and theoretical study is being carried out, to obtain fundamental understanding of the processing-structure-property relationship of ceramic epitaxial film and multilayers prepared by chemical vapor deposition technique. The participants will usually join a research project in progress and become involved, depending on the participants interest and training, with either experimental or theoretical techniques described above.

315 RADIATION AND KINETICS EFFECTS

Mat. Sci.
Metal. Engr.
Nucl. Engr.
Phy.

Fundamental mechanisms which induce microstructural changes during irradiation are studied. Investigations of surface modifications by ion beams are directed toward understanding processes (such as ion beam mixing, radiation-enhanced interdiffusion, and sputtering) that produce surface layers with properties significantly different from those of bulk material. Research on radiation-induced segregation and defect production is providing a fundamental basis for the engineering of materials tailored to specific applications in both fission and fusion radiation environments. Additional studies focus on fundamental properties, defects, and irradiation effects in high Tc superconductors.

Emphasis is placed on experimental techniques which allow quantitative information about microstructural changes to be obtained in situ, e.g, ion beam analysis, Auger depth-profiling, and conventional and analytical electron microscopy. Computer and analytical modeling are used in support of the experimental activities.

316 AMORPHOUS ALLOYS AND NANOCRYSTALLINE MATERIALS

Chem.
Engr. Phy.
Mat. Sci.
Metal. Engr.
Nucl. Engr.
Phy.

Amorphous and nanocrystalline alloys are relatively new classes of materials that have unique and often useful properties not found with normal coarse-grained polycrystalline materials. We prepare these materials by thermal evaporation, solid-state reaction of nanocrystalline powders and thin films, melt spinning and ion irradiation. We have begun studies of nanocrystalline ceramics, which show markedly improved properties; e.g, they sinter to high densities at relatively low temperatures. Characterization involves the study (by electron microscopy and its ancillary techniques: XEDS, EELS, etc.) of the nucleation of metastable phases at crystalline interfaces, of crystallites in amorphous phases; and of the nature of the atomic structure of the interface regions by x-ray diffraction, HREM, and EXAFS measurements (by resistometry, x-ray and neutron diffraction, Brillouin scattering, and calorimetry) of the transformation kinetics of solid-state and ion-induced reactions; mechanical property changes; and the modeling of physical processes such as interdiffusion and irradiation. Participants will be assigned a specific project which could involve the preparation of materials and/or running experiments for the characterization of these materials.

317 ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

Ceram.
Comp. Sci.
Elec. Engr.
Mat. Sci.
Metal. Engr.
Nucl. Engr.
Phy.

Research in the Electron Microscopy Center is directed toward the experimental determination of the morphology, crystallography, elemental, chemical composition, and electronic structure of phases, interfaces, surfaces and defects present in pure elements, alloys, ceramics and other technologically important materials. State-of-the-art transmission and scanning transmission electron microscopes (TEM/STEM's) as well as a 1.2 MeV high voltage electron microscope (HVEM) are employed to characterize the microstructure of solids using conventional diffraction contrast techniques. Quantitative analytical information is obtained through the use of x-ray energy dispersive and electron energy loss spectrometers for elemental, chemical, and electronic structure studies interfaced to these instruments. This analytical information is obtainable from regions which can be as small as 10 nanometers in diameter. Investigators can choose to concentrate on applications of transmission electron microscopy based techniques to characterize materials, or research on fundamental (experimental or theoretical) studies of electron/solid interactions to advance state-of-the-art understanding and techniques for characterization. When appropriate, joint appointments between the Electron Microscopy Center and various MSD research groups will be suggested.

318 INTERFACE STUDIES

Ceram.
Chem.
Mat. Sci.
Nucl. Engr.
Phy.

The basic physical properties of solid interfaces are investigated by means of experimental and computer-simulation methods. The atomistic simulation methods (which involve lattice statics and dynamics, molecular dynamics and Monte-Carlo techniques) are aimed at determining, for example, the structure and free energy of interfaces as a function of temperature, their point-defect properties (such as impurity segregation and diffusion), and the properties of voids in grain boundaries and in the bulk. Phenomena investigated experimentally include the atomistic structure and properties of grain boundaries in metals, semiconductors and ceramics as well as interphase boundaries between them, atomic transport, and impurity segregation. The experimental methods applied include high-resolution and analytical electron microscopy, SIMS, Rutherford backscattering and radiotracer diffusion. Participants are invited to contribute to a variety of theoretical and/or experimental programs related to the basic understanding of solid interfaces.

319 LASERS IN SURFACE SCIENCE

Chem.
Mat. Sci.
Phy.

Several orders of magnitude increases in detection sensitivity of adsorbed species are achievable by making use of laser ionization of neutral atoms and molecules emitted from surfaces by ion, electron-or photo-stimulated desorption. The rational underlying the effort is that for most systems the desorbed neutral/ion ratios are very large, typically 103-105, and that laser ionization in contradistinction to other ionization methods can approach 100% efficiency. Recent advances in instrumentation take advantage of sophisticated developments in angle and energy refocusing time-of-flight mass spectrometric detection, advanced electronic pulsing and timing circuitry, and extensive computer control of instrument operation so that useful yields for sputtered atoms near 5% of the sputtered flux can now be obtained.

Future directions include extensive studies of the sputtering yield behavior of a variety of materials in the low damage regime; exploiting the element-specific nature of resonance multiphoton ionization to solve problems in geochemistry where isobaric interferences play havoc with, for example, the Ru-Os chronometer; measuring for the first time electron- and photon-induced neutral desorption yields; elucidating the mechanism of optical damage in materials, by bringing to bear our ultrasensitive detection methods at very low bombarding laser fluxes and fluences.

320 SURFACE SEGREGATION IN DILUTE METAL ALLOYS

Chem.
Mat. Sci.
Metal. Engr.
Phy.

Surface segregation in dilute alloys (e.g., Cu-Li) is being studied under ion bombardment conditions by a variety of surface spectroscopies (Auger, X-ray photoemission, UV photoemission, ion scattering and secondary ion mass spectroscopy). The purpose is to understand processes which make it possible to produce materials in which the surface properties are significantly different from those of the bulk, and to apply the techniques developed to limiter and first-wall problems in magnetic-confinement fusion devices.

321 MOLECULAR SIEVE MATERIALS--HETEROGENEOUS CATALYSTS

Chem.
Engr.
Mat. Sci.
Phy.
Theory

Molecular sieve materials in the aluminosilicate zeolite family and the newer aluminophosphate and silicoaluminophosphate families are being synthesized. Basic mechanistic aspects of their crystallization from gels are being investigated. Characterizations and studies of basic properties of these materials and their modifications are undertaken with a variety of techniques, including x-ray diffraction and spectroscopy, electron microscopy, neutron small-angle and inelastic scattering, nuclear magnetic resonance and electron paramagnetic resonance spectroscopies. Atom-atom theoretical calculations and molecular dynamics computer simulation methods are being applied to study molecular interactions and adsorbate diffusion in the intracrystalline pores. These characteristics dictate shape-selective adsorption and catalytic properties. Cation siting and ion exchange are being studied with magnetic resonance spectroscopy. Sieve material modification by incorporation of nanometer-sized metallic particles to effect shape-selective catalysis by metal is being explored.

322 INTERFACIAL MATERIALS CHEMISTRY

Chem.
Comp. Sci.
Envr. Sci.
Phy.
Theory

A novel fully-automated thin-film sputter-deposition system has been developed for the preparation of stoichiometrically exact and reproducible high-Tc thin films. This system is a unique combination of a single ion or laser beam desorption source and multiple elemental targets. The thin films will be characterized using modern surface analytical instrumentation. In other work, EMF measurements of the partial pressures of oxygen as a function of oxygen stoichiometry have been made on $YBa_2Cu_3O_x$ for x = 6.2 to 6.9 and at temperatures ranging from 400 to 750 C. Extrapolation of the log Po2 versus x plots to lower temperatures is consistent with the presence of a miscibility gap at < 290 C in the orthorhombic phase field. Such a gap had been predicted by us on the basis of extended Hückel cluster calculations. In new ab initio molecular orbital calculations of copper oxide clusters representing $YBa_2Cu_3O_x$, it was found that oxygen hole (0-1) formation is favored energetically over Cu^{3+} and that holes occur in p rather than s-type orbitals. These findings have important implications for the mechanism of superconductivity in these materials. Our results also suggest that the inequivalent oxygens in the 1-2-3 compound give rise to low-lying electronic excitations near 0.4 eV which had been experimentally observed in optical reflectivity studies.

The thrust of a newly initiated program is to elucidate the mechanisms of action and to develop techniques to control the effect of additives on polymers. Polymers are complex molecular mixtures whose performance depends critically on additives such as plasticizers, ultraviolet sensitizers, fungicides, lubicants, corrosion inhibitors, and adhesion promoters, for example. The studies involve resonance ionization of desorbed neutral molecules followed by Fourier transform mass spectroscopy and are aimed at determining the surface and near-surface concentration of additives under a variety of conditions.

323 AQUEOUS CORROSION

Chem.
Math.
Metal.
Phy.
Theory

This project undertakes basic research aimed at elucidating fundamental aspects of aqueous corrosion under conditions of temperature and pressure (300 C, 10 MPA) relevant to fission reactor environments. Mechanisms responsible for passivation on iron and nickel-based alloys and for crack and pit propagation in these same alloys are being investigated. The details that connect surface adsorption, electron transfer, and electrolyte chemistry with passive film structure are sought by a combination of in situ surface sensitive spectroscopic methods and transient electrochemical techniques. Strong emphasis is placed on both ambient and high-temperature studies of processes occurring at metal/electrolyte and oxide/electrolyte interfaces and on concurrent research to formulate and test first principle corrosion models. In situ measurements using laser Raman, Raman-gain, and second harmonic generation spectroscopies provide information on the structure of species at metal/solution interfaces. Key features of the interfacial chemistry associated with passivation processes (including charge transfer kinetics) are being studied by pulsed galvanostatic/potentiostatic, dc polarization, and ac impedance techniques. A parallel theoretical effort seeks to simulate solid/liquid interface phenomena through the application of molecular dynamics methods in combination with ab initio molecular orbital theory.

324 THERMODYNAMICS OF ORDERED AND METASTABLE MATERIALS

Chem.
Comp. Sci.
Math.
Phy.

In this project, experimental and theoretical studies are carried out to investigate important thermodynamic and structural properties of ordered solutions, amorphous (metastable) materials, strategic minerals, and chemical species that have significance for elevated-temperature corrosion processes. Fundamental thermodynamic measurements (e.g., emf) are combined with structural (e.g., neutron diffraction) and theoretical (e.g., molecular dynamics) studies to probe the solution behavior of ordered and associated liquids (e.g., chloroaluminates, "ionic" alloys, silicates). Efforts are under way to extend this research to include Mössbauer and Extended X-ray Absorption Fine Structure studies of the bonding properties of ordered phases at very low temperatures, i.e., below 25K. Thermodynamic calculations based on statistical mechanical methods are applied to the computation of the thermodynamic characteristics of complex metallurgical media as well as corrosion processes. Electronic absorption spectroscopy and a variety of other physiochemical techniques, including X-ray diffraction, proton activation, and cyclic voltammetry are used to explore the dissolution of metals contained in domestic minerals and in industrial/energy by-products. Thermodynamical techniques are employed to determine enthalpies of formation, standard entropies, and Gibbs energies of formation of strategically important minerals, fiber optic materials, and fast ion conducting glasses. Drop calorimetric and vapor pressure measurements are made on systems exhibiting metal-to-nonmetal transitions to develop a sound fundamental understanding of this important phenomenon.

Basic superconductivity is being studied in the Materials Science Division. Seen here collaborating on this effort are two undergraduates, two graduate students, a faculty member and an Argonne senior scientist.

MATHEMATICS AND COMPUTER SCIENCE DIVISION (MCS)

The Mathematics and Computer Science Division carries out basic research in advanced computing, applied analysis, computational mathematics, and software methodology.

ADVANCED COMPUTING

Advanced Computing research emphasizes the creation of portable algorithms and software for computers with advanced architectures, the development of parallel programming methodologies, the study of parallel programming languages, and applications of advanced computing in biology and climate modeling.

325 PARALLEL PROGRAMMING ENVIRONMENTS

Comp. Sci. Investigations involve design of parallel programming environments, parallel programming methodologies, and graphical tools for parallel program analysis.

326 ALGORITHMS AND SOFTWARE

Comp. Sci. Research involves the design and implementation of algorithms for advanced computers. Emphasis is placed on fundamental computations. Areas include linear equations, linear least squares, matrix eigenvalues, and optimization.

Math.

327 PARALLEL PROGRAMMING METHODOLOGIES

Comp. Sci. Investigations involve design of methods to coordinate the complex synchronization patterns of multiprocessors, and development of new measurement techniques to study performance issues in parallel programs.

328 PARALLEL PROGRAMMING LANGUAGES

Comp. Sci. Logic programming languages such as Prolog and Strand, as well as computer languages such as Ada, are evaluated as languages for parallel programming.

329 APPLICATIONS OF ADVANCED COMPUTING IN BIOLOGY

Comp. Sci. Research focuses on applications of parallel computation and logic programming to sequence comparison, secondary structure determination, and gel analysis.

330 AUTOMATIC DIFFERENTIATION

Comp. Sci. Research focuses on computing exact gradients and Jacobians of multivariate functions on parallel architectures and integrating them into an application framework.

331 PARALLEL CLIMATE MODELING

Comp. Sci. Research focuses on the development of programming methodologies, algorithms, and graphics tools to support climate modeling on large parallel machines.

Math.

332 HIGH-LEVEL PARALLEL PROGRAMMING

Comp. Sci. Research is concerned with techniques that simplify parallel programming by providing more abstract, high-level programming notations. Topics include the design and implementation of high-level parallel languages (Strand and PCN), bilingual programming, compiler development, and techniques for reusing parallel program components.

APPLIED ANALYSIS

Applied Analysis research involves the application of analytical and numerical techniques to problems in the natural and engineering sciences.

333 BIFURCATION PHENOMENA

Math. Research focuses on the analysis of bifurcation phenomena in fluid flow, reaction-diffusion systems, and combustion. Numerical methods are also used in the analysis of these phenomena.

334 NONLINEAR DIFFERENTIAL EQUATIONS

Math. Studies involve the qualitative analysis of nonlinear differential equations.

335 SYMBOLIC MANIPULATION

Comp. Sci. Computer software that can perform exact algebraic and analytic calculations is used to study various mathematical problems arising in applied mathematics. Topics include combustion, differential equations, matrix theory, and robotics.

Math.

336 COMPUTATIONAL FLUID DYNAMICS

Comp. Sci. Efforts focus on the development and evaluation of numerical procedures for fluid flow and gas dynamics problems. Current investigations address the shallow water equation and the primitive equations for global climate studies.

Math.

COMPUTATIONAL MATHEMATICS

Computational Mathematics involves the design of numerical algorithms and techniques for preparing and evaluating software.

337 OPTIMIZATION

Comp. Sci. Research centers on the development of algorithms and software for the solution of large-scale nonlinear optimization problems. Participants will work on projects that include the incorporation of automatic differentiation techniques in optimization

Math. software, the implementation on parallel computers of simulated annealing and genetic algorithms for combinatorial and nonlinear problems, and the development of trust region and gradient project methods for large-scale problems.

338 APPROXIMATIONS AND SOFTWARE BASICS

Comp. Sci.

Math.

Efforts involve design and analysis of algorithms for (1) approximation of functions, (2) special and elementary function calculations, and (3) testing function software. The theoretical aspects emphasize convergence and accuracy analysis of the algorithms; the practical aspects emphasize implementation of the algorithms in highly accurate and portable software.

339 QUADRATURE

Math.

Recent investigations have focused on lattice rules for high-dimensional quadrature, series acceleration techniques, and problems involving Laplace and Fourier transforms. Various projects involve well-defined problems ranging from the highly theoretical (Does a rule having a particular specification exist?) to the practical (Which rule does a better job in a particular environment?).

340 NUMERICAL SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS

Comp. Sci.

Math.

Investigation focuses on the use of preconditioning techniques in conjunction with conjugate gradient methods for solving nonlinear systems of partial differential equations.

SOFTWARE METHODOLOGY

The Software Methodology activity focuses on problems that are involved in developing and using computer software.

341 AUTOMATED REASONING

Comp. Sci.

Math.

Investigations are under way to develop new concepts and new applications for automated reasoning and to investigate the value and use of parallelism. Participants are offered the opportunity to formulate more effective ways of reasoning (inference rules), devise more powerful strategies to control the reasoning, and study various applications - which include answering open questions from mathematics, designing and validating circuits, and proving properties of computer programs. The opportunity also exists for widening the scope of automated reasoning by discovering totally new uses for programs that reason logically. With the object of extending the effectiveness of automated reasoning programs, our activities also include the analysis and design of complex systems built from interconnected components.

342 SOFTWARE TOOLS AND PROGRAMMING ENVIRONMENTS

Math.

Comp. Sci.

Research focuses on the creation of Fortran-oriented software tools that aid in adapting existing Fortran programs to run on vector and parallel machines. Tools are written in an extension of Fortran and form part of a programming environment that provides various analysis and transformation capabilities.

343 VISUALIZATION IN SCIENTIFIC COMPUTATION

Comp. Sci.

This work is concerned with developing interactive graphical tools to aid in the development of numerical methods and the interpretation of the results of computations. Most of this work is done with the X window system in order to provide a portable set of tools. Of particular interest is the use of animation as a way of providing insight into a computation.

344 AUTOMATED PROGRAM TRANSFORMATION

Comp. Sci.

Investigations seek to simplify and automate the production of efficient programs from high-level specifications. Participants can investigate such topics as the suitability of functional programming, logic programming, and object-oriented programming for specifying both numerical and nonnumerical algorithms. In addition, they can study ways to derive efficiently executable programs from such specifications. Finally, they can automate their derivations using program transformations and the TAMPR program transformation system.

Our current investigations center on deriving efficient programs for parallel computers, such as the Encore Multimax, Sequent Balance, and the Thinking Machines Connection Machine. Participants do not need to know how to write transformations or specifications. However, they should be interested in the process of writing programs and be excited by the prospect of seeing the computer write programs by following the directions they give it.

OFFICE OF PUBLIC AFFAIRS (OPA)

345 OFFICE OF PUBLIC AFFAIRS INTERNSHIP

Journ.

Publ. Rel.

Sci. Writing

The Office of Public Affairs has internship opportunities for students interested in science related journalism and public relations. The student would do "hands-on" activities in many of the areas of the Office of Public Affairs, including: the preparation of news releases reporting on scientific and technical advances at Argonne; assisting in the publication of the Argonne Week, and the Argonne News (employee publications), and logos, a quarterly scientific review; aiding in the planning and management of scientific conferences; and becoming conversant with the activities of Argonne's award winning motion picture and video group. This internship requires a strong background in journalism and an interest in science. Articles generated during the internship are printed in Argonne publications with author credit, and used in news release form to scientific and general media.

Encouraging students to pursue research careers in science and engineering is an important component of Argonne's mission. Featured speakers at a career symposium for the more than 400 participants in Argonne summer programs were Drs. Alan Schriesheim, Laboratory Director, Mildred Dresselhaus, Institute Professor at The Massachusetts Institute of Technology, and Leon Lederman, former director of Fermi National Accelerator Laboratory and recipient of the 1988 Nobel Prize in Physics.

PHYSICS DIVISION (PHY)

The Physics Division conducts basic experimental and theoretical research in nuclear physics and atomic and molecular physics. We are also involved in the continuing development of a novel superconducting heavy-ion accelerator called ATLAS, which is operated as a national facility for nuclear physics research.

346 SUPERCONDUCTING HEAVY-ION LINAC "ATLAS"

Phy.

Engr.

Construction of the world's first superconducting heavy-ion accelerator is complete. This project has involved the development of a new technology. Operation of the accelerator will involve continuing upgrading tasks that are concerned with surface phenomena in r.f. resonators, cryogenic design, computer control, and the refinement of mechanical subsystems. Research participants could be involved with computer control of equipment and other aspects of accelerator development. A new upgrade of ATLAS has begun. The project goal is to replace the injector Tandem accelerator with a new low-velocity profile superconducting linear accelerator and an electron-cyclotron-resonance ion source.

347 NUCLEAR REACTIONS INDUCED BY HEAVY IONS

Phy.

The interaction between nuclei is studied. Collisions are observed between accelerated heavy ions from the superconducting linac (at present to mass » 100 and a maximum beam energy close to 1 GeV) and target nuclei over the full periodic table. These studies involve: Elastic and inelastic scattering, heavy-ion resonances, nucleon transfer between colliding nuclei, compound nucleus formation and fusion, particle and fission decay, gamma decay of high-spin states, nuclear astrophysics, and the production of nuclei far off stability. In addition, the full accelerator system is used as an ultrasensitive mass spectrometer for radioisotope detection at very low concentrations, with applications in various areas of physics and related research fields. Research participants could be involved in one or more of the experimental aspects of these studies which include, in addition to the accelerator system, particle detection techniques with solid-state and gas detectors, magnetic spectrometers and ion beam optics, gamma-ray semiconductor detectors, picosecond time-of-flight, thin-foil target techniques, high-vacuum technology, multiparameter pulse electronics and computer data handling and analysis.

348 NUCLEAR PHYSICS AT INTERMEDIATE ENERGIES

Phy.

The strong interaction in nuclear matter is explored in these studies. In particular, meson and quark effects as well as other sub-nucleonic features of nuclei are studied primarily with leptonic probes. Experiments are performed at the newly-commissioned muon laboratory at Fermilab, the Stanford Linear Accelerator Center and the MIT-Bates Linear Accelerator Laboratory. Novel particle detector arrays, a computer-based (VAX 11-750) data acquisition system and a laser driven polarized target are examples of the equipment being developed for these studies.

349 EXPERIMENTS WITH THE FRAGMENT MASS ANALYZER

Phy.

This project involves using the new Fragment Mass Analyzer (FMA) for various nuclear reaction studies. One example is measurements of the masses and decay properties of radioactive nuclei, in particular those of interest to astrophysics. They are produced using the ATLAS heavy ion accelerator, and the FMA is used to separate the desired isotopes for observation. Other experiments will study the gamma rays emitted by nuclei possessing very high angular momenta. The FMA will be used to select the desired nucleus out of the many that are produced.

350 NUCLEAR ASTROPHYSICS REACTIONS

Phy. Nuclear reactions of interest to astrophysics are being studied using accelerators in the Physics Division. Of current interest now are the properties of a Br81 solar neutrino detector.

351 WEAK INTERACTIONS

Phy. This area of research concentrates on aspects of the fundamental weak interaction and extensions to the standard model of the forces of nature. Previous research as well as ongoing projects investigate the manifestation of the weak force in nuclei: consequences of the conserved-vector-current hypothesis (CVC); the extent of validity of the principle of partially-conserved axial currents (PCAC); parity mixing in nuclei due to the neutral weak current; and precision measurements of weak-interaction parameters. An ongoing experiment at the Institute Laue-Langevin (ILL) in Grenoble, France studies the weak decay parameters of the neutron Experiments are also undertaken to look for signals of physics beyond the standard model: a search for neutrino oscillation; searches for axions; a light Higgs particle search. Experiments are carried out at the Argonne Dynamitron and Tandem accelerators, nearby university tandem laboratories, the Los Alamos Meson Physics Facility (LAMPF), and the ILL in France.

352 THEORETICAL PHYSICS

Phy. Most of our theoretical physics research concentrates on the nuclear many-body problem, pion-nucleon-nucleon interactions and heavy-ion reactions, and the development of numerical computational techniques for nuclear physics. Particular attention has been given to interactions of nuclei with pions, leptons, nucleons, and heavier ions. We also carry out theoretical research in relativistic particle theory and in atomic physics.

EXPERIMENTAL ATOMIC AND MOLECULAR PHYSICS

The experimental atomic and molecular physics research in the Physics Division is centered around four main programs.

353 BEAM-FOIL SPECTROSCOPY

Phy. Precision measurements are being made on radiation emitted by highly-stripped ions of 2 or 3 electrons in order to test calculations of relativistic and quantum-electrodynamic effects. Studies of radiation from multi-excited positive and negative ions are underway as systems of interest for x-ray laser development.

354 FAST (MeV) MOLECULAR IONS

Phy. Argonne's 4.5-MV Dynamitron and tandem-LINAC accelerators are used to study the interactions of fast (MeV) atomic and molecular ions with matter. The project has as its main objective a general study of the interactions of fast charged particles with matter, but with the emphasis on those aspects that take advantage of the unique features inherent in employing molecular-ion beams (e.g., the feature that each molecular ion incident upon a solid target forms a tight cluster of atomic ions that remain correlated in space and time as they penetrate the target). Additionally, these techniques have allowed the direct determination of the geometrical structures of molecular ions.

355 HIGH-RESOLUTION SPECTROSCOPY WITH TUNABLE LASERS AND ATOMIC AND MOLECULAR BEAMS

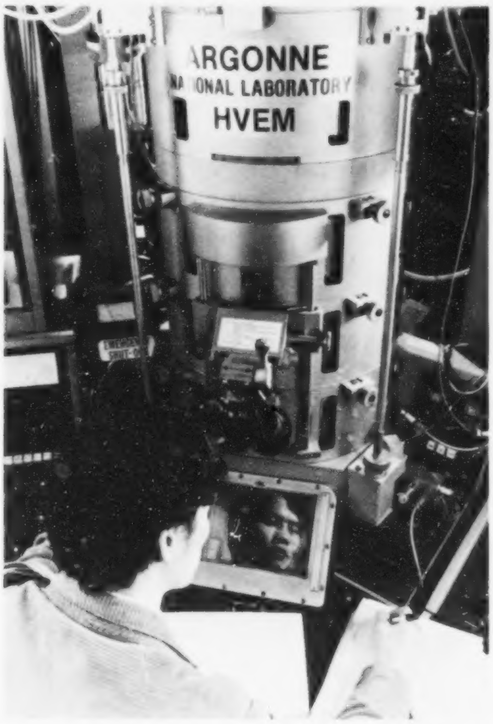
Phy. An atomic-beam apparatus is used for high-resolution laser-fluorescence studies of atoms and molecules. In addition, laser rf double-resonance techniques are used to study hyperfine structure and isotope shifts. A new apparatus with collinear laser and ion beams is under construction to allow similar studies of slow atomic and molecular ions.

356 ION-PHOTON INTERACTIONS

Phy. Measurements are made on interactions of intersecting beams of fast ions from an accelerator and photons from an intense tunable laser. The project has a variety of objectives; e.g., the laser spectroscopy of exotic ionic species, studies on collisional excitation (in foils or gases) from non ground-state atomic species, etc.

357 ATOMIC PHYSICS AT ATLAS

Phy. Atomic physics studies are underway at ATLAS, Argonne's heavy-ion accelerator that is capable of generating intense high-quality beams of a wide variety of atomic ions with energies variable up to about 10 MeV/nucleon. X-ray, optical and electron spectroscopic studies on highly ionized species are conducted as well as a wide range of other atomic physics research.



Students in Argonne's Summer Research Participation Program examine a target area for the Argonne Tandem Linac Accelerator System or ATLAS.

REACTOR ANALYSIS AND SAFETY DIVISION (RAS)

This Division develops analytical methods and experimental techniques needed to ensure reactor safety. The effort encompasses the analysis of potential accidents, reactor control, coolant dynamics, core structural safety, fuel-element damage propagation, fuel dynamics, fuel-coolant interactions, heat transfer, and engineered safety features (such as containment).

To improve understanding of the safety of liquid-metal-cooled reactors (LMRs) and light water-cooled reactors (LWRs) and heavy-water-cooled reactors (HWRs), the Division conducts research and development to identify technology needs; investigates safety questions and related phenomena; develops safety data, design methods, and criteria; and recommends appropriate safety philosophies.

358 ANALYSIS OF IN-PILE EXPERIMENTS

Chem. Engr.

Comp. Sci.

Elec. Engr.

In-reactor experiments are performed and analyzed to provide a data base for reactor safety analyses on response of fuel, cladding, fission products, and coolants to severe transient heating. Opportunities exist for research in analyzing instrumentation response; thermal behavior of fuel and coolant; detailed response of fuel, fission-products, and cladding through gross melting and movement; and energy transfer between components. The project is divided between analyses/planning of future tests, and analysis of previous experiments.

Math. *Mech. Engr.* *Metal Engr.* *Nucl. Engr.* *Phy.*

359 NUCLEAR DIAGNOSTICS

Comp. Sci.

Elec. Engr.

Nucl. Engr.

Phy.

Experiments in the reactor safety program are routinely instrumented with nuclear-radiation detectors. The Experimental Physics Section makes use of the fast neutron hodoscope to image fuel and structure motion and of other neutron and gamma instruments to detect specific properties of radiating substances. Participants from many technical disciplines have been involved in design, calculations, detector development, nuclear effects, electronics, data processing, image reconstruction and analysis and other areas. Although the hodoscope is operated at TREAT reactor in Idaho, data processing and all other support are carried out at ANL-East. Hardware at TREAT consists of a multichannel collimator, 360 neutron and gamma detection channels, and electronics for signal processing, temporary storage, and data recording. To generate final results, steps involved next are data recovery, processing algorithms, image reconstruction and plotting, and analysis. A micro VAX is used in timesharing and interactive modes. Studies are proceeding on new instrumentation, methods of image analysis, corrections for system effects, and new applications of radiation imaging technology.

360 LARGE-SCALE COMPUTER CODE DEVELOPMENT

Comp. Sci.
Math.
Mech. Engr.
Nucl. Engr.

Large-scale computer codes for the analysis of operational and accidental transients in liquid metal-cooled reactor (LMR) systems are developed. Activities include (1) development of understanding of basic physical phenomena, (2) formulation of mathematical models, (3) development of numerical solution techniques for coupled, non-linear partial differential equation systems, (4) computer code programming (FORTRAN) and verification, (5) code and modeling validation (experiment analysis), and (6) code performance, improvement, maintenance, and graphics.

Model development and validation requires proficiency in heat transfer, single and two-phase fluid dynamics, reactor physics (kinetics), and engineering mechanics. Computer code development activities include numerical analysis methods, programming, and code verification and maintenance.

361 COMPUTER STUDIES OF IFR CORES

Comp. Sci.
Math.
Nucl. Engr.

Analyses are performed to predict the behavior of liquid metal-cooled reactor (LMR) systems in operational and accidental transients. Large-scale computer codes containing models of heat transfer, single and two-phase flow, reactor neutron kinetics, and structural-mechanical behavior are employed. The participant should have a basic understanding of heat transfer and fluid flow and a working knowledge of FORTRAN. Experience with large-scale scientific computer codes and applications is desirable.

362 FUEL BEHAVIOR

Engr. Mech.
Mat. Sci.
Metal.
Nucl. Engr.

This project is aimed at developing an understanding of the behavior of nuclear reactor fuel and fuel materials under reactor accident conditions. Models of phenomena governing material behavior are sought, as are ways of integrating these models into computer codes to predict fuel behavior under severe transient heating. Current emphasis is on modeling of metallic fuels and advanced alloy cladding. Opportunities are available in model development, finite element code development and experimental mechanics and metallurgy. Fundamental studies of fission product behavior in nuclear fuels are also of interest.

363 HEAT TRANSFER AND FLUID DYNAMICS

Chem. Engr.
Comp. Sci.
Mech. Engr.
Phy.

Analytical, experimental and fundamental studies are being performed on a wide variety of heat transfer and fluid dynamics phenomena relevant to nuclear reactor safety assessment. Areas currently under active investigation include two-phase flow modeling for LWR, safety analysis, basic studies on two-phase flow pattern and interfacial area, liquid-liquid explosions including vapor explosions, liquid metal combustion, and radiative heat transfer in two-phase mixtures. High-speed motion picture cameras and a flash x-ray system are available for experimental work.

364 TOMOGRAPHY

Chem. Engr.
Comp. Sci.
Elec. Engr.
Math.
Mech. Engr.

Tomographic reconstructions of reactor fuel cross-sections are developed, using, as basic data, neutron radiographs taken at many angles. (Current analyses use 75 angles, with an angular separation of 2.4 degree). The radiographs are digitized, and the digitized information is processed by a set of computer programs developed at Argonne to normalize, align and filter the data and to produce digital representations of cross-sections at selected elevations. These digital representations are converted to false-color and gray-scale images on video monitors and hard-copy devices. This technique provides a non-invasive, non-destructive alternative to the usual destructive examination of a spatial distribution of fuel-bearing material. In some cases, this technique can eliminate the need for time-consuming destructive post-test examinations. In other cases, where destructive examinations are required to obtain metallography information, tomography can be used in the planning of the destructive examinations, to make them as time- and cost-effective as possible.

Metal. Engr. *Nucl. Engr.* *Phy.*

365 COMPUTER STUDIES IN ENGINEERING MECHANICS PROGRAM

Civil Engr.
Engr. Mech.
Mech. Engr.
Nucl. Engr.

The program primarily involves the development and validation of analytical models and computer codes for safety analysis associated with core mechanics, reactor vessels and structures, and containment analysis. Background and interest in fluid-structure interaction, thermomechanical analysis, seismic studies, (including fluid-structure interaction and seismic isolation), buckling analysis, and prestressed or high-temperature concrete applications of engineering mechanics are desirable. Strong skills in numerical analysis, finite element methods and computer programming, preferably in large structural computer codes, are needed. Mathematical formulations and computer codes are to be developed for such tasks as (a) primary system response analysis, (b) core subassembly response analysis, (c) three-dimensional analysis of complicated LMR structures, e.g., reactor head covers, (d) response of heat transport system piping and associated components, (e) seismic analysis, (f) reinforced and prestressed concrete reactor vessels and containment structures, and (g) high-temperature response of concrete structures.

366 PROBABILISTIC RISK ASSESSMENT

Comp. Sci.
Elec. Engr.

Probabilistic Risk Assessment (PRA) areas include: Methods development and applications in PRA of energy systems including consequence analysis; probabilistic methods and applications in nuclear plant and/or reactor accident analysis; computer software reliability assessment; sensitivity theory methods and applications in PRA; systems reliability modeling with common cause emphasis; and cost benefit analysis.

Math. *Mech. Engr.* *Nucl. Engr.*

367 ARTIFICIAL INTELLIGENCE (AI) BASED PLANT CONTROL SYSTEMS

Advances in the field of AI and work on inherently safe plant designs have resulted in the possibility of reactor plant automation to such a degree that a knowledge data base could be utilized through the use of online computers. Automated reasoning codes for plant process diagnostics and control will be required for this particular application of AI systems. Establishment of a generic methodology to develop these codes for plant operation utilizing AI techniques and tools such as PROLOG/LISP and expert system shells will be the focus of this research area. Issues involved in the application of these automated reasoning techniques to safe reactor operation will require resolution. Access to the automated reasoner capability at Argonne National Laboratory's Mathematics and Computer Science Division is a possibility. Methodology developed will be tested in conjunction with the EBR-II Division at the EBR-II reactor.

Comp. Sci. *Elec. Engr.* *Mech. Engr.* *Nucl. Engr.*

368 LIGHT WATER REACTOR SAFETY ANALYSIS

A number of studies are under way involving various aspects of nuclear reactor technology. These include studies of foreign reactor systems, studies of U.S. plant features, and modeling of the physical processes of postulated reactor accidents. The modeling activities closely coincide with ongoing laboratory experimental programs studying accident phenomena. The thermal-hydraulic, chemical interaction, and aerosol behavior of the real or simulated core melt materials are modeled in computer routines. The participants work with staff who are developing the physical models, creating computer routines, and integrating the computer models into large-scale, integrated computer codes.

Aeros. Sci. *Chem. Engr.* *Comp. Sci.* *Mech. Engr.* *Nucl. Engr.* *Phy.*

369 REACTOR SAFETY LABORATORY EXPERIMENTS

Laboratory tests are performed to improve our understanding of the phenomena of postulated severe accidents at nuclear reactors. Some of the programs aim at quantifying the risk of present day reactors while others are aimed at demonstrating passive means to avoid accident consequences for future reactors. The experiments have been addressing such phenomena as core degradation, aerosol formation and transport (source term), melting/freezing phenomena, multi-fluid mixing, vapor explosions, quench and coolability of high-temperature heat-generating debris, chemical reactions, and interactions with concrete. Participants will work with staff members who are conducting these tests and will gain practical experience in laboratory techniques, equipment, safety practices, and interpretation and modeling of results. Of particular value is the hands-on experience with instrumentation used for pressure, temperature, and flowrate measurements; with data acquisition equipment such as analog and digital recorders, fibre-optic visicorders, motion picture photography, and high-speed video recording; and with computers and software used for data processing, plotting, and reports.

Aeros. Sci. *Chem. Engr.* *Comp. Sci.* *Elec. Engr.* *Mech. Engr.* *Nucl. Engr.* *Phy.*

370 DECAY HEAT REMOVAL

Laboratory experiments on advanced passive decay heat removal systems are being performed. Programs involve large passive natural air convection decay heat removal systems and natural convection boiling water heat transfer decay heat removal systems. Participants will work with staff members who are conducting these tests and will gain practical experience in laboratory techniques, equipment, safety practices, and interpretation and modeling of results.

371 QUANTITATIVE IMAGE ANALYSIS

Post-test examination of nuclear fuels, which have undergone reactor-accident simulations, makes use of quantitative metallography performed on a PC-based image analysis system. The participant will use the system to measure metallurgical features observed in micrographs from optical microscopes and secondary electron images produced by scanning electron microscopes.

Comp. Sci.
Elec. Engr.
Mat. Sci.   *Mech. Engr.*   *Metal.*   *Nucl. Engr.*

372 ARMS CONTROL TREATY VERIFICATION AND NATIONAL SECURITY

The technologies developed in research often have useful application in verifying arms control treaties and other non-military national security applications, such as detection of contraband smuggling. Examples of technologies currently under development for both nuclear and non-nuclear treaty verification (such as START, CWC, CFE, CTB) are hodoscope-related radiation detection instruments, neutron and gamma detectors, accelerators, electronic systems, and scanning-electron microscopes. These are to be applied to counting missile reentry vehicles, measuring rocket-motor diameters, detecting nuclear warheads, determining chemical composition, or uniquely tagging military items. The objects of interest might have fissionable materials, high-explosives, chemical agents, or other substances. Opportunities exist for contributions at any level in analysis, computations, and experiments, depending on current national concerns and on the experience and interests of the program participant.

Chem. Engr.
Comp. Sci.
Elec. Engr.
Mat. Sci.
Math.   *Nucl. Engr.*   *Phy.*

373 EXPERIMENTAL BREEDER REACTOR (EBR-II) SUPPORT

The primary mission for EBR-II is to support the Integral Fast Reactor (IFR) concept for advanced liquid metal reactors (LMR). EBR-II conducts programs for metal fuel development and concept key-feature testing. This reactor is also the U.S. Department of Energy's prime facility for irradiation of fuels and materials in the LMR development program. The EBR-II Division is located at Argonne West (Idaho), and the EBR-II Support sections are located in the RAS and EP Divisions in Illinois.

374 ARTIFICIAL INTELLIGENCE (AI) BASED PLANT DIAGNOSTICS AND CONTROL SYSTEMS

Advances in the field of AI and work on inherently safe plant designs have resulted in the possibility of reactor plant automation to such a degree that a knowledge data base could be utilized through the use of on-line computers. Automated reasoning codes, in the form of expert systems, for plant process diagnostics and control will be required for this particular application. Establishment of a generic methodology to develop knowledge bases and inference mechanisms for these diagnostic/control systems will be the focus of this research area. Specifically, research will consist of the representation of "deep" knowledge of the plant processes, including structural and functional knowledge, first-principle physical laws and qualitative and quantitative modeling. AI techniques and tools such as PROLOG/LISP languages and expert systems shells will be used in the development of such systems. Methodology developed will be tested in conjunction with the EBR-II Division at the EBR-II reactor.

TECHNOLOGY TRANSFER CENTER (TTC)

The Technology Transfer Center is the focus for transferring Argonne technology to industry and for cooperative programs with industry. The Center's activities include:

- Evaluating Argonne's inventions for commercial potential.
- Transferring technology developed by Argonne to private industry.
- Publicizing Argonne's inventions, patents, unique facilities and expertise.
- Providing access to technical and other specialized assistance to private industry.
- Facilitating the formation of "spin-off" companies started by Argonne personnel.
- Developing cooperative initiatives with industries, universities, economic development institutions, and state and federal governments.
- Developing data bases on Argonne technologies, facilities, and skills.

Studies and assessments will be conducted on the mechanisms for transferring technology to the marketplace, evaluation of existing programs, documentation of case histories and development of techniques for marketing Argonne's unique skills. Studies will be conducted under the supervision of TTC staff members. Participants will also assist staff members on data bases, marketing studies for new inventions, and assisting new business start-ups.

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